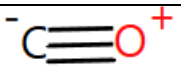
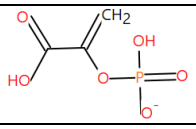
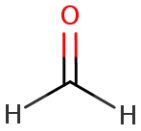
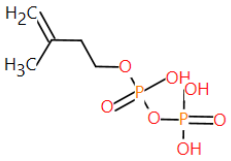
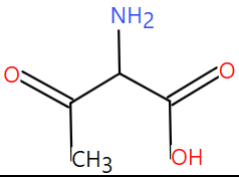
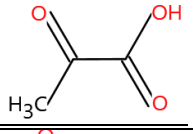
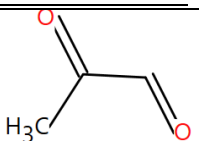
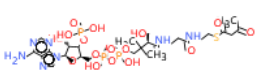
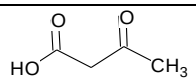
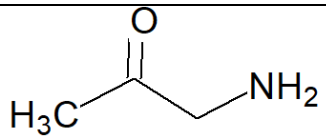
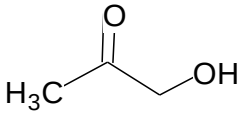
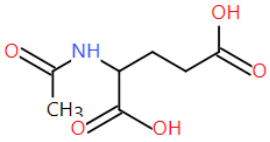
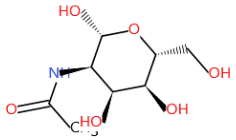
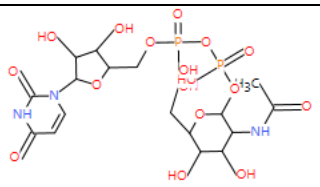
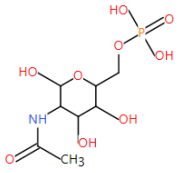
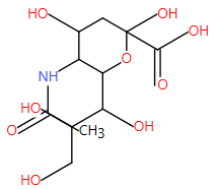
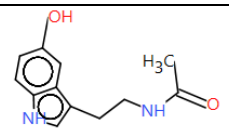
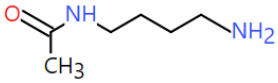
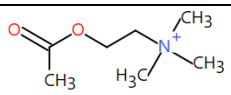
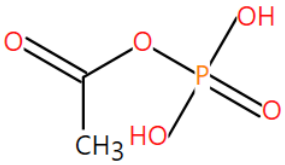
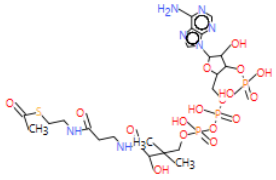
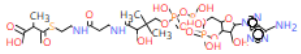
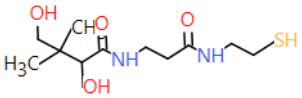
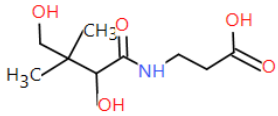
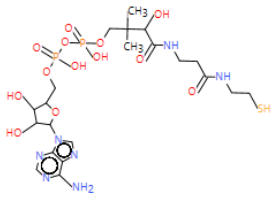
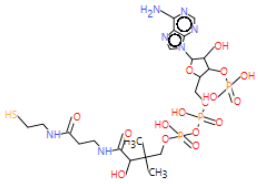
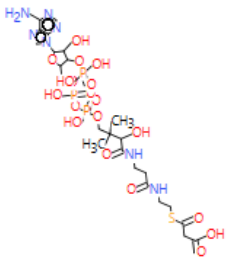
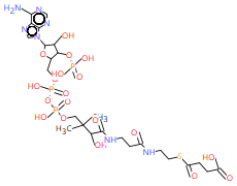
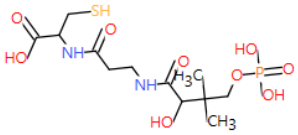
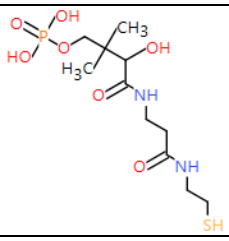
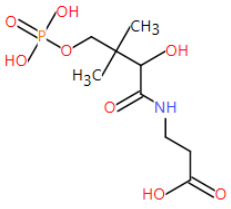
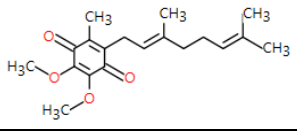
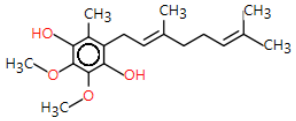
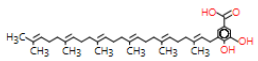
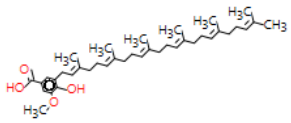
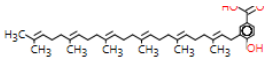
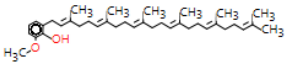
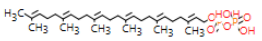
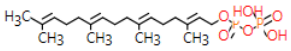
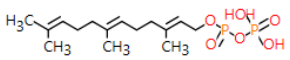
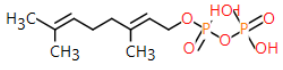
Appendix 1: List with 429 predefined chemicals included in the definition of Q1: Is the substance a normal constituent of the body (F) or an optical isomer of such?

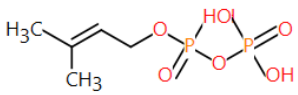
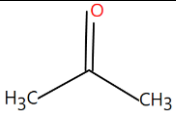
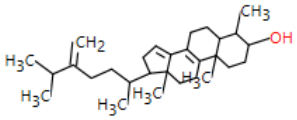
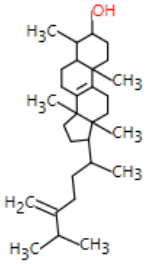
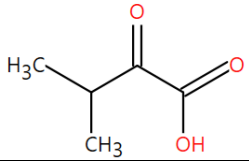
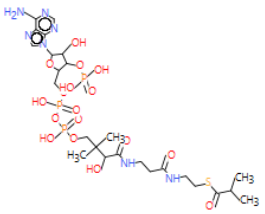
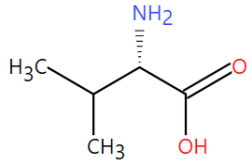
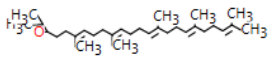
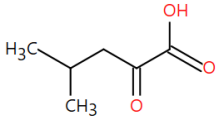
#	CAS #	EC #	Chemical name	SMILES	Structure	Reference source
1	7783-07-5	231-978-9	Hydrogen selenide	[SeH2]		https://biocyc.org/compound?orgid=HUMAN&id=CPD-678
2	630-08-0	211-128-3	Carbon monooxide	[C-]#[O+]		http://biocyc.org/HUMAN/NEW-IMAGE?object=CARBON-MONOXIDE
3	73-89-2		Phosphoenolpyruvate	OC(=O)C(=C)OP(O)([O-])=O		
4	50-00-0	2000018	Formaldehyde	C=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=FORMALDEHYDE
5			DELTA3-ISOPENTENYL-PP	CC(=C)CCOP(=O)(O)OP(=O)(O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=DELTA3-ISOPENTENYL-PP
6			AMINO-OXOBUT	CC(=O)C(N)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=AMINO-OXOBUT
7	127-17-3	2048243	Pyruvate	CC(O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=PYRUVATE
8	78-98-8	2011648	METHYL-GLYOXAL	CC(=O)C=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=METHYL-GLYOXAL
9	1420-36-6	2158159	Acetoacetyl-CoA	[H]C3(COP(=O)(O)OP(=O)(O)OCC(C)(C)C(O)C(=O)NCCC(=O)NCCSC(=O)CC(C)=O)(OC([H])(N		http://biocyc.org/HUMAN/NEW-IMAGE?object=ACETOACETYL-COA

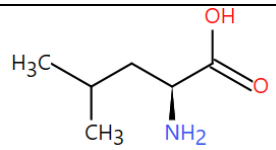
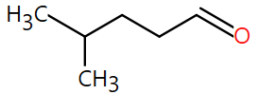
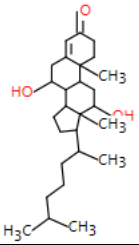
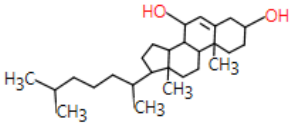
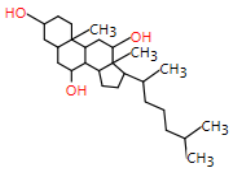
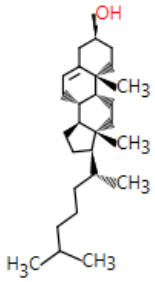
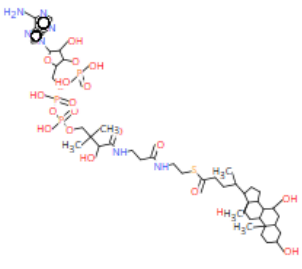
				2C=NC=1C(N)=NC=NC=12)C([H])(O)C3([H])(OP(=O)(O)O))		
10	541-50-4		3-Ketobutyrate	CC(=O)CC(=O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=3-KETOBUTYRATE
11	298-08-8		Amino-acetone	CC(=O)CN		http://biocyc.org/HUMAN/NEW-IMAGE?object=AMINO-ACETONE
12	116-09-6	204-124-8	Acetol	CC(=O)CO		http://biocyc.org/HUMAN/NEW-IMAGE?object=ACETOL
13	1188-37-0		ACETYL-GLU	CC(=O)NC(CCC(O)=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=ACETYL-GLU
14	31022-50-1		Acetylgalactosamine	CC(=O)N[C@H]1C(O)O[C@H](CO)[C@H](O)[C@@H]1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD-3604
15	528-04-1		UDP-N-Acetyl-D-Glucosamine	CC(=O)NC1C(O)C(O)C(CO)OC1OP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1O)N1C=CC(=O)NC1=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=UDP-N-ACETYL-D-GLUCOSAMINE
16	102029-88-9		N-ACETYL-D-GLUCOSAMINE-6-P	CC(=O)NC1C(O)OC(COP(O)(O)=O)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=N-ACETYL-D-GLUCOSAMINE-6-P
17	131-48-6		N-ACETYLNEURAMINATE	CC(=O)NC1C(O)CC(O)(OC1C(O)C(O)CO)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=N-ACETYLNEURAMINATE

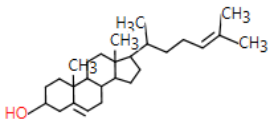
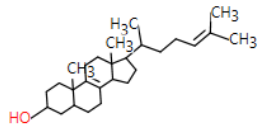
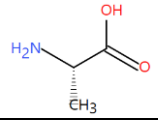
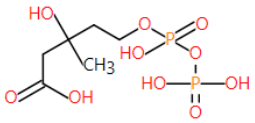
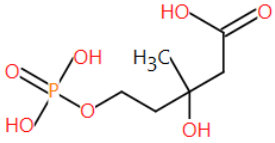
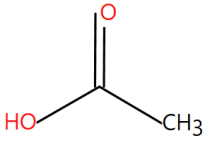
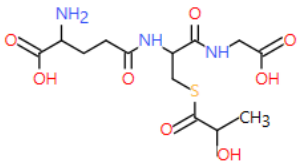
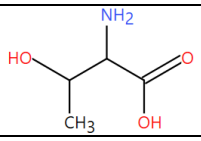
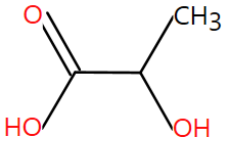
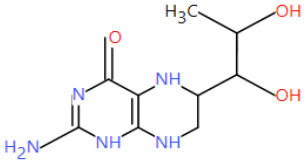
18	1210-83-9		N-Acetylserotonin	CC(=O)NCCc1c[nH]c2ccc(O)cc12		
19	18233-70-0		CPD-569	CC(=O)NCCCCN		
20	51-84-3		Acetylcholine	CC(=O)OCC[N+](C)(C)C		http://biocyc.org/HUMAN/NEW-IMAGE?object=ACETYLCHOLINE
21			L-Glutamate-5-P	CC(=O)OP(O)(O)=O		
22	72-89-9		Acetyl-COA	CC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12		
23	104809-02-1		D-Methyl-malonyl-COA	CC(C(O)=O)C(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12		
24	496-65-1		CPD-511	CC(C)(CO)C(O)C(=O)NCCC(=O)NCCS		
25	79-83-4		Pantothenate	CC(C)(CO)C(O)C(=O)NCCC(O)=O		
26	3633-59-8		DEPHOSPHO-COA	CC(C)(COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1O)n1cnc2c(N)ncnc12)C(O)C(=O)NCCC(=O)NCCS		

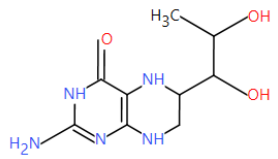
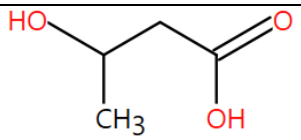
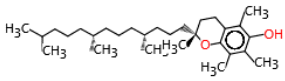
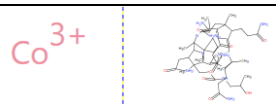
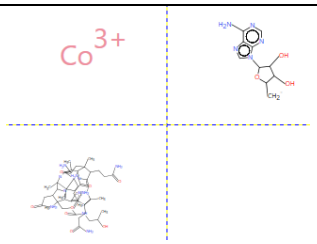
27	85-61-0		CO-A	CC(C)(COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc21)C(O)C(=O)NCCC(=O)NCCS		
28			MALONYL-COA	CC(C)(COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12)C(O)C(=O)NCCC(=O)NCCSC(=O)CC(O)=O		
29	604-98-8		SUC-COA	CC(C)(COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12)C(O)C(=O)NCCC(=O)NCCSC(=O)CCC(O)=O		
30			R-4-PHOSPHOPANTOTHENOYL-L-CYSTEINE	CC(C)(COP(O)(O)=O)C(O)C(=O)NCCC(=O)NC(CS)C(O)=O		
31			PANTETHEINE-P	CC(C)(COP(O)(O)=O)C(O)C(=O)NCCC(=O)NCCS		
32			4-P-PANTOTHENATE	CC(C)(COP(O)(O)=O)C(O)C(=O)NCCC(O)=O		
33	1339-63-5		UBIQUINONE-8	COC1C(=O)C(C)=C(CC=C(C)CCC=C(C)C)C(=O)C=1OC		

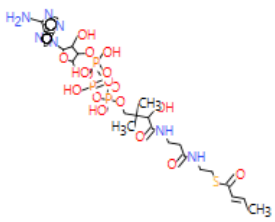
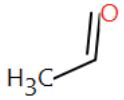
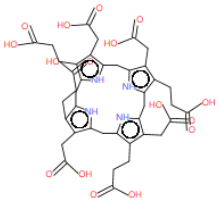
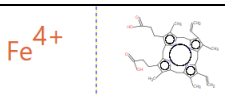
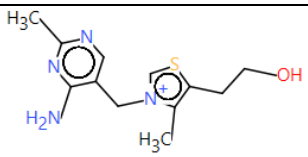
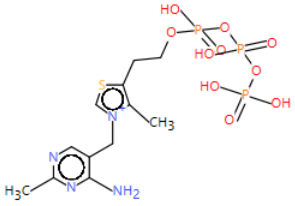
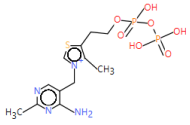
34			UBIQUINOL-8	COc1c(O)c(C)c(CC=C(C)CCC=C(C)C)c(O)c1OC		
35			3-HEXAPRENYL-45-DIHYDROXYBENZOATE	COc1cc(cc(CC=C(C)CCC=C(C)CCC=C(C)CCC=C(C)CCC=C(C)CCC=C(C)C)c1O)C(O)=O		
36			3-HEXAPRENYL-4-HYDROXY-5-METHOXYBENZOATE	COc1cc(cc(CC=C(C)CCC=C(C)CCC=C(C)CCC=C(C)CCC=C(C)CCC=C(C)C)c1O)C(O)=O		
37			3-HEXAPRENYL-4-HYDROXYBENZOATE	CC(C)=CCCC(C)=CCCC(C)=CCCC(C)=CCCC(C)=CCCC(C)=CCc1cc(ccc1O)C(O)=O		
38			2-HEXAPRENYL-6-METHOXYPHENOL	COc1cccc(CC=C(C)CCC=C(C)CCC=C(C)CCC=C(C)CCC=C(C)C)c1O		
39			ALL-TRANS-HEXAPRENYL-DIPHOSPHATE	CC(C)=CCCC(C)=CCCC(C)=CCCC(C)=CCCC(C)=CCOP(O)(=O)OP(O)(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=ALL-TRANS-HEXAPRENYL-DIPHOSPHATE
40			GERANYLGERANYL-PP	CC(C)=CCCC(C)=CCCC(C)=CCCC(C)=CCOP(O)(=O)OP(O)(O)=O		
41	13058-04-3		FARNESYL-PP	CC(C)=CCCC(C)=CCCC(C)=CCOP(O)(=O)OP(O)(O)=O		
42			GERANYL-PP	CC(C)=CCCC(C)=CCOP(O)(=O)OP(O)(O)		

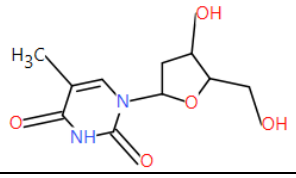
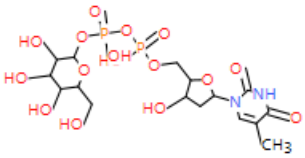
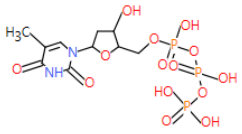
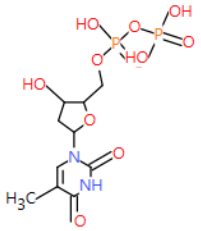
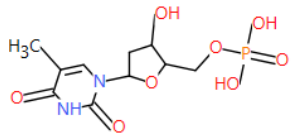
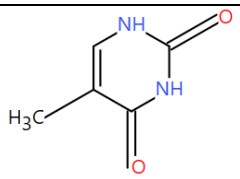
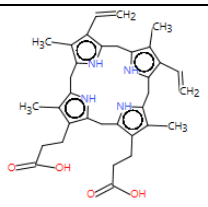
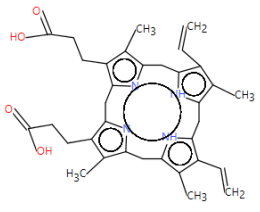
				=O		
43	358-71-4		CPD-4211	CC(C)=CCOP(O)(=O)OP(O)(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD-4211
44	67-64-1		ACETONE	CC(C)=O		
45			ALPHA-METHYL-5-ALPHA-ERGOSTA	CC(C)C(=C)CCC(C)C1CC=C2C3CCC4C(C)C(O)CCC4(C)C=3CCC12C		
46			Obtusifoliol	CC(C)C(=C)CCC(C)C1CCC2(C)C3CCC4C(C)C(O)CCC4(C)C=3CCC12C		http://biocyc.org/HUMAN/NEW-IMAGE?object=OBTUSIFOLIOL
47	759-05-7		2-KETO-ISOVALERATE	CC(C)C(=O)C(O)=O		
48	15621-60-0		ISOBUTYRYL-COA	CC(C)C(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12		
49	72-18-4		VALINE	CC(C)[C@H](N)C(O)=O		
50	9029-62-3		EPOXYSQUALENE	CC(C)=CCCC(C)=CCCC(C)=CCCC=C(C)CCC=C(C)CCC1OC1(C)C		
51	816-66-0		2K-4CH3-PENTANOATE	CC(C)CC(=O)C(=O)O		

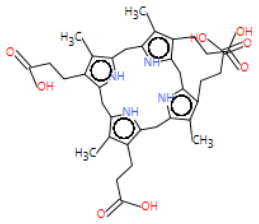
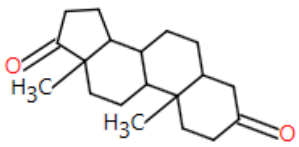
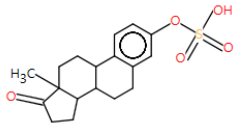
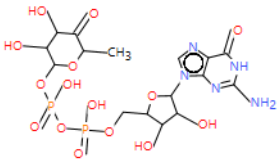
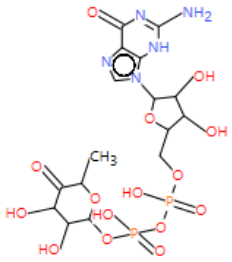
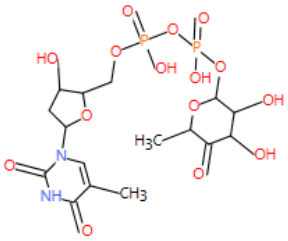
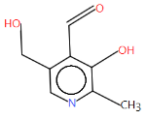
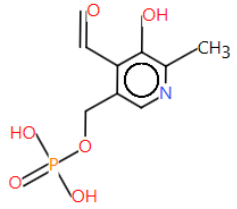
52	61-90-5		LEUCINE	CC(C)C[C@H](N)C(O)=O		
53	1119-16-0		4-METHYLPENTANAL	CC(C)CCC=O		
54			CPD-1087	CC(C)CCCC(C)C1CCC2C3C(O)CC4=CC(=O)CCC4(C)C3CC(O)C12C		
55			CPD-266	CC(C)CCCC(C)C1CCC2C3C(O)C=C4CC(O)CCC4(C)C3CCC12C		
56			5-BETA-CHOLESTANE-3-ALPHA7-ALPHA12-ALP	CC(C)CCCC(C)C1CCC2C3C(O)CC4CC(O)CCC4(C)C3CC(O)C12C		
57		57-88-5	CHOLESTEROL	[H][C@@]1(CC[C@]2([H])[C@]1(C)CC[C@]3([H])[C@@]4(C)CC[C@H](O)CC4=CC[C@@]23[H])[C@H](C)CCCC(C)C		
58			CPD-202	CC(CCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc21)C1CCC2C3C(O)CC4CC(O)CCC4(C)C3CC(O)C12C		

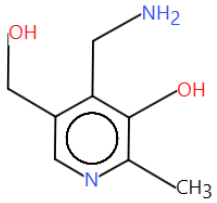
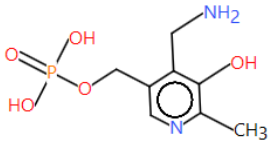
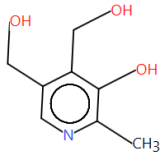
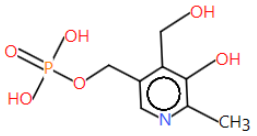
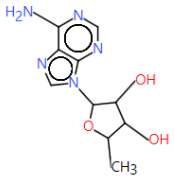
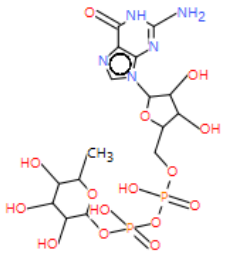
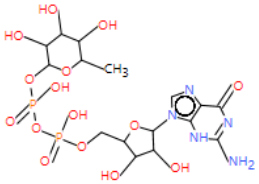
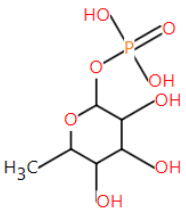
59	313-04-2		DESMOSTEROL-CPD	CC(CCC=C(C)C)C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C		
60	128-33-6		ZYMOSTEROL	CC(CCC=C(C)C)C1CCC2C3CCC4CC(O)CCC4(C)C=3CCC12C		
61	56-41-7		ALANINE	C[C@H](N)C(O)=O		
62	4872-34-8		CPD-641	CC(O)(CCOP(O)(=O)OP(O)(O)=O)CC(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD-641
63	73566-35-5		CPD-499	CC(O)(CCOP(O)(O)=O)CC(O)=O		
64	71-50-1		ACET	CC(=O)O		
65	25138-66-3		S-LACTOYL-GLUTATHIONE	CC(O)C(=O)SCC(NC(=O)CCC(N)C(O)=O)C(=O)NCC(O)=O		
66	72-19-5		THREONINE	CC(O)C(N)C(O)=O		
67	10326-41-7	2011962	D-LACTATE	CC(O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=D-LACTATE
68	17528-72-2		5,6,7,8-Tetrahydrobiopterin;TETRA-H-BIOPTERIN_2	CC(O)C(O)C1CNC2NC(N)=NC(=O)C=2N1		http://biocyc.org/HUMAN/NEW-IMAGE?object=TETRA-H-BIOPTERIN

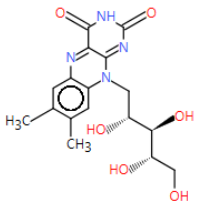
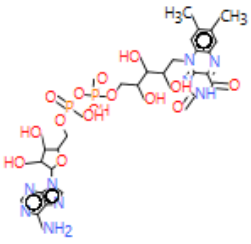
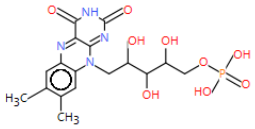
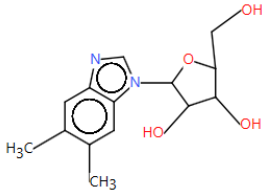
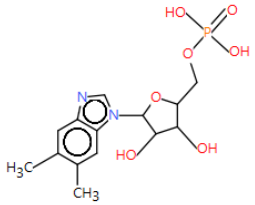
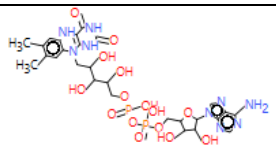
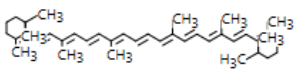
69	17528-72-2		TETRA-H-BIOPTERIN	CC(O)C(O)C1CNC2N=C(N)NC(=O)C=2N1		http://biocyc.org/HUMAN/NEW-IMAGE?object=TETRA-H-BIOPTERIN
70	625-72-9		CPD-335	[H]C(C)(O)CC(=O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD-335
71	59-02-9	2004122	Vitamin E	CC(C)CCC[C@@H](C)CCC[C@@H](C)CCC[C@]1(C)CCc2c(C)c(O)c(C)c(C)c2O1		https://www.tandfonline.com/doi/abs/10.1080/10629360802083871
72	1867-62-5		COBINAMIDE	CC(O)CNC(=O)CCC1(C)C(CC(N)=O)C2N=C1C(C)=C1N=C(C=C3N=C(C(C)=C4[N-]C2(C)C(C)(CC(N)=O)C4CCC(N)=O)C(C)(CC(N)=O)C3CCC(N)=O)C(C)(C)C1CCC(N)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=COBINAMIDE
73			ADENOSYLCOBINAMIDE	[Co+3].[CH2-]C1OC(C(O)C1O)n1cnc2c(N)ncnc21.CC(O)CNC(=O)CCC1(C)C(CC(N)=O)C2N=C1C(C)=C1N=C(C=C3N=C(C(C)=C4[N-]C2(C)C(C)(CC(N)=O)C4CCC(N)=O)C(C)(CC(N)=O)C3CCC(N)=O)C(C)(C)C1CCC(N)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=ADENOSYLCOBINAMIDE
74	102680-35-3		CROTONYL-COA	CC=CC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)		http://biocyc.org/HUMAN/NEW-IMAGE?object=CROTONYL-COA

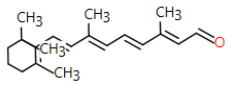
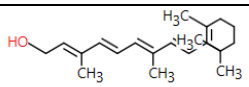
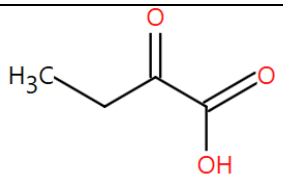
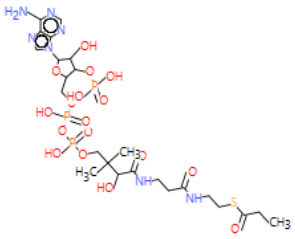
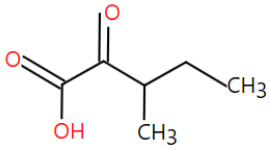
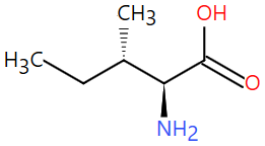
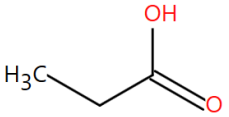
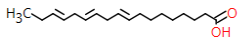
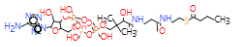
				(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12		
75	75-07-0	75-07-02008368	ACETALD	CC=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=ACETALD
76	1976-85-8		UROPORPHYRINOGEN-III	OC(=O)CCc1c2Cc3[nH]c(Cc4[nH]c(Cc5[nH]c(Cc([nH]2)c1CC(O)=O)c(CCC(O)=O)c5CC(O)=O)c(CCC(O)=O)c4CC(O)=O)c(CC(O)=O)c3CCC(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=UROPORPHYRINOGEN-III
77	14875-96-8		PROTOHEME	[Fe+4].Cc1c(CCC(O)=O)c2cc3[n-]c(cc4nc(cc5[n-]c(cc1n2)c(C)c5C=C)c(C)c4C=C)c(C)c3CCC(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=PROTOHEME
78	59-43-8		Thiamine	Cc1ncc(C[n+]2csc(CCO)c2C)c(N)n1		http://biocyc.org/HUMAN/NEW-IMAGE?object=THIAMINE
79	15666-52-1		CPD-611	Cc1ncc(C[n+]2csc(CCOP(O)(=O)OP(O)(=O)OP(O)(O)=O)c2C)c(N)n1		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD-611
80	154-87-0		THIAMINE-PYROPHOSPHATE	CC2=NC=C(C[N+]1=CSC(CCO)=C1(C))C(N)=N2		http://biocyc.org/HUMAN/NEW-IMAGE?object=THIAMINE

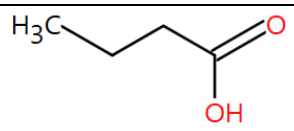
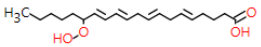
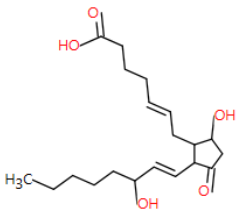
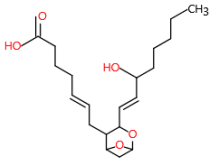
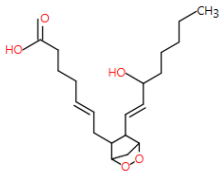
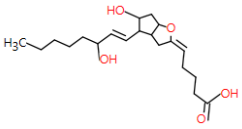
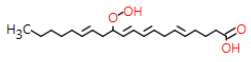
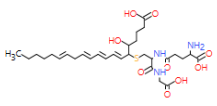
81	50-89-5		THYMIDINE	CC1=CN(C2CC(O)C(CO)O2)C(=O)NC1=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=THYMIDINE
82	2009-24-7		DTDP-D-GLUCOSE	CC1=CN(C2CC(O)C(COP(O)(=O)OP(O)(=O)OC3OC(CO)C(O)C(O)C3O)O2)C(=O)NC1=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=DTDP-D-GLUCOSE
83			Deoxythymidine triphosphate	CC1=CN(C2CC(O)C(COP(O)(=O)OP(O)(=O)OP(O)(O)=O)O2)C(=O)NC1=O		
84			Deoxythymidine diphosphate	CC1=CN(C2CC(O)C(COP(O)(=O)OP(O)(O)=O)O2)C(=O)NC1=O		
85			Deoxythymidine monophosphate	CC1=CN(C2CC(O)C(COP(O)(O)=O)O2)C(=O)NC1=O		
86	65-71-4		THYMINE	CC1=CNC(=O)NC1=O		
87	7412-77-3		Protoporphyrinogen	Cc1c2Cc3[nH]c(Cc4[nH]c(Cc5[nH]c(Cc([nH]2)c1CCC(O)=O)c(CCC(O)=O)c5C)c(C=C)c4C)c(C=C)c3C		http://biocyc.org/HUMAN/NEW-IMAGE?object=PROTOPORPHYRINOGEN
88	553-12-8		PROTOPORPHYRIN_IX	Cc1c(CCC(O)=O)c2cc3nc(cc4[nH]c(cc5[nH]c(cc1n2)c(C)c5C=C)c(C)c4C=C)c(C)c3CCC(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=PROTOPORPHYRIN_IX

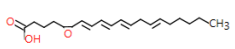
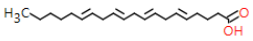
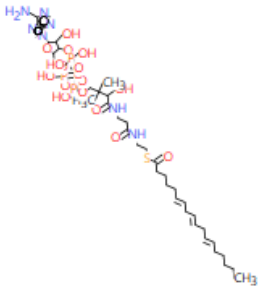
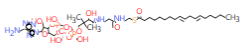
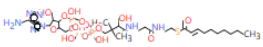
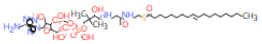
89	2624-63-7		COPROPORPHYRINOGEN_III	Cc1c2Cc3[nH]c(Cc4[nH]c(Cc5[nH]c(Cc([nH]2)c1CCC(O)=O)c(C)c5CCC(O)=O)c(C)c4CCC(O)=O)c(CCC(O)=O)c3C		http://biocyc.org/HUMAN/NEW-IMAGE?object=COPROPORPHYRINOGEN_III
90	846-46-8	2126855	CPD-342	CC12CCC(=O)CC1CCC1C2CCC2(C)C1CCC2=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD-342
91	481-97-0		ESTRONE-SULFATE	CC12CCC3C(CCc4cc(OS(O)(=O)=O)ccc34)C1CCC2=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=ESTRONE-SULFATE
92			GDP-4-DEHYDRO-6-DEOXY-D-MANNOSE	CC1OC(OP(O)(=O)OP(O)(=O)OCC2OC(C(O)C2O)n2cnc3C(=O)NC(N)=Nc32)C(O)C(O)C1=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=GDP-4-DEHYDRO-6-DEOXY-D-MANNOSE
93			GDP-4-DEHYDRO-6-DEOXY-D-MANNOSE_2	CC1OC(OP(O)(=O)OP(O)(=O)OCC2OC(C(O)C2O)n2cnc3C(=O)N=C(N)Nc32)C(O)C(O)C1=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=GDP-4-DEHYDRO-6-DEOXY-D-MANNOSE
94			DTDP-DEOH-DEOXY-GLUCOSE	CC1OC(OP(O)(=O)OP(O)(=O)OCC2OC(CC2O)N2C=C(C)C(=O)NC2=O)C(O)C(O)C1=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=DTDP-DEOH-DEOXY-GLUCOSE
95	66-72-8	2006308	PYRIDOXAL	CC1=NC=C(CO)C(C=O)=C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=PYRIDOXAL
96	54-47-7		PYRIDOXAL_PHOSPHATE	Cc1ncc(COP(O)(O)=O)c(C=O)c1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=PYRIDOXAL_PHOSPHATE

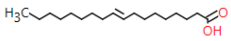
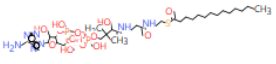
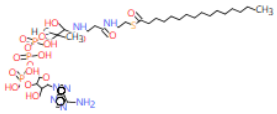
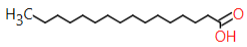
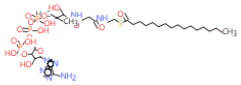
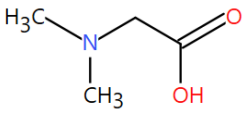
97	85-87-0	2016405	PYRIDOXAMINE	Cc1ncc(CO)c(CN)c1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=PYRIDOXAMINE
98	529-96-4	2084716	PYRIDOXAMINE-5P	Cc1ncc(COP(O)(O)=O)c(CN)c1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=PYRIDOXAMINE-5P
99	65-23-6	2006030	PYRIDOXINE	Cc1ncc(CO)c(CO)c1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=PYRIDOXINE
100	447-05-2	2071796	PYRIDOXINE-5P	Cc1ncc(COP(O)(O)=O)c(CO)c1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=PYRIDOXINE-5P
101			CH33ADO	CC1OC(C(O)C1O)n1cnc2c(N)ncnc12		http://biocyc.org/HUMAN/NEW-IMAGE?object=CH33ADO
102	15839-70-0		GUANOSINE_DIPHOSPHATE_FUCOSE_2	CC1OC(OP(O)(=O)OP(O)(=O)OCC2OC(C(O)C2O)n2cnc3C(=O)NC(N)=Nc23)C(O)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=GUANOSINE_DIPHOSPHATE_FUCOSE
103	15839-70-0		GUANOSINE_DIPHOSPHATE_FUCOSE	CC1OC(OP(O)(=O)OP(O)(=O)OCC2OC(C(O)C2O)n2cnc3C(=O)N=C(N)Nc23)C(O)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=GUANOSINE_DIPHOSPHATE_FUCOSE
104	526-31-8		CPD-488	CC1OC(OP(O)(O)=O)C(O)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD-488
105	83-88-5		RIBOFLAVIN	Cc1cc2N=C3C		

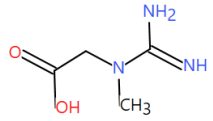
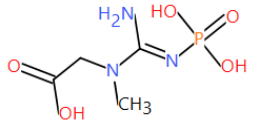
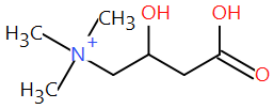
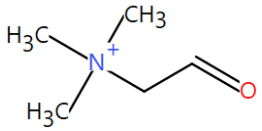
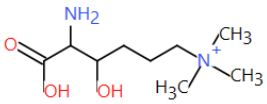
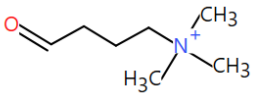
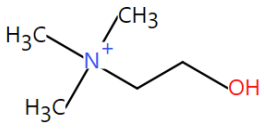
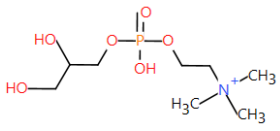
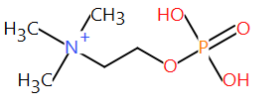
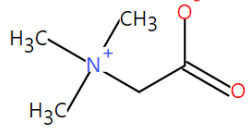
				(=O)NC(=O)N=C3N(C[C@@H](O)[C@@H](O)[C@@H](O)CO)c2cc1C		
106	146-14-5	2056631	FAD	Cc1cc2N=C3C(=O)NC(=O)N=C3N(CC(O)C(O)C(O)COP(O)(=O)OP(O)(=O)OCC3OC(C(O)C3O)n3cnc4c(N)ncnc34)c2cc1C		http://biocyc.org/HUMAN/NEW-IMAGE?object=FAD
107	146-17-8		C17H21N4O9P	Cc1cc2N=C3C(=O)NC(=O)N=C3N(CC(O)C(O)C(O)COP(O)(O)=O)c2cc1C		http://biocyc.org/HUMAN/NEW-IMAGE?object=FMN
108			alpha-Ribazole	Cc1cc2ncn(C3OC(CO)C(O)C3O)c2cc1C		http://biocyc.org/HUMAN/NEW-IMAGE?object=ALPHA-RIBAZOLE
109			ALPHA-RIBAZOLE-5-P	Cc1cc2ncn(C3OC(COP(O)(O)=O)C(O)C3O)c2cc1C		http://biocyc.org/HUMAN/NEW-IMAGE?object=ALPHA-RIBAZOLE-5-P
110	1910-41-4		FADH2	Cc1cc2NC3C(=O)NC(=O)NC=3N(CC(O)C(O)C(O)COP(O)(=O)OP(O)(=O)OCC3OC(C(O)C3O)n3cnc4c(N)ncnc43)c2cc1C		http://biocyc.org/HUMAN/NEW-IMAGE?object=FADH2
111	7235-40-7		CPD1F-129	CC(C=CC=C(C)C=CC1=C(C)CCCC1(C)C)=CC=CC=C(C)C=CC=C(C)C=CC1=C(C)CCCC1(C)C		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD1F-129

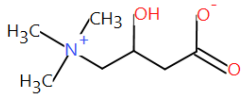
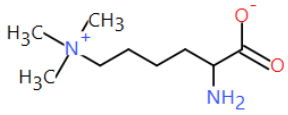
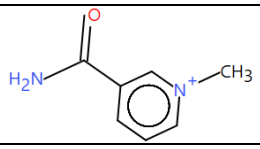
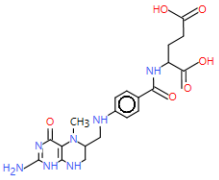
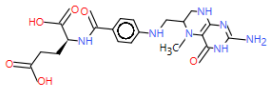
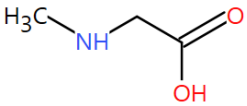
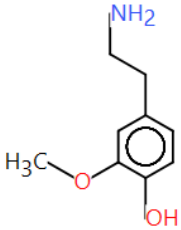
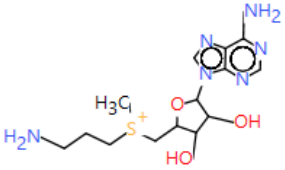
112	116-31-4		RETINAL	CC(C=CC=C(C)C=CC1=C(C)CCCC1(C)C)=CC=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=RETINAL
113	11103-57-4		Retinol	CC(C=CC=C(C)C=CC1=C(C)CCCC1(C)C)=CCO		http://biocyc.org/HUMAN/NEW-IMAGE?object=RETINOL
114	600-18-0	2099869	2-OXOBUTANOATE	CCC(=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=2-OXOBUTANOATE
115	317-66-8		PROPIONYL-COA	CCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc21		http://biocyc.org/HUMAN/NEW-IMAGE?object=PROPIONYL-COA
116	1460-34-0	2159550	2-KETO-3-METHYL-VALERATE	CCC(C)C(=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=2-KETO-3-METHYL-VALERATE
117	73-32-5		Isoleucine	CC[C@H](C)[C@H](N)C(O)=O		
118	79-09-4	2011763	PROPIONATE	CCC(=O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=PROPIONATE
119	463-40-1		LINOLENIC_ACID	CCC=CCC=CCC=CCCCCCCCC(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=LINOLENIC_ACID
120	2140-48-9		BUTYRYL-COA	CCCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12		http://biocyc.org/HUMAN/NEW-IMAGE?object=BUTYRYL-COA

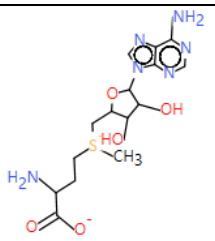
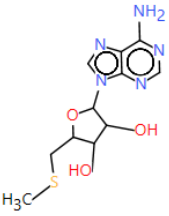
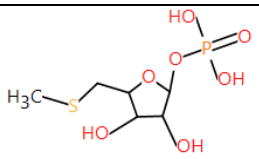
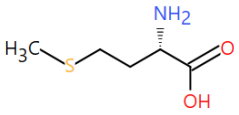
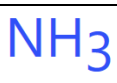
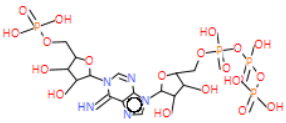
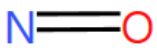
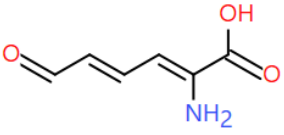
121	107-92-6	2035323	BUTYRIC_ACID	CCCC(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=BUTYRIC_ACID
122			5Z8Z11Z13E-15S-15-HYDROPEROXYICOS	CCCCCC(OO)C=CC=CCC=CCC=CCCCC(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=5Z8Z11Z13E-15S-15-HYDROPEROXYICOS
123	41598-07-6		5Z13E-15S-9-ALPHA15-DIHYDROXY-11-O	CCCCCC(O)C=CC1C(CC=CCCCC(O)=O)C(O)CC1=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=5Z13E-15S-9-ALPHA15-DIHYDROXY-11-O
124			ALPHA11-ALPHA-EPOXY-15-HYDROXYTHROMBA	CCCCCC(O)C=CC1OC2CC(O2)C1CC=CCCCC(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=ALPHA11-ALPHA-EPOXY-15-HYDROXYTHROMBA
125	42935-17-1		PROSTAGLANDIN-H2	CCCCCC(O)C=CC1C2CC(OO2)C1CC=CCCCC(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=PROSTAGLANDIN-H2
126	35121-78-9		5Z13E-15S-69-ALPHA-EPOXY-11-ALPHA	CCCCCC(O)C=CC1C(O)CC2OC(CC12)=CCCCC(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=5Z13E-15S-69-ALPHA-EPOXY-11-ALPHA
127			5Z8Z10E14Z-12S-12-HYDROPEROXYICOS	CCCCCC=CCC(OO)C=CC=CCC=CCCCC(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=5Z8Z10E14Z-12S-12-HYDROPEROXYICOS
128	72025-60-6		LEUKOTRIENE-C4	CCCCCC=CCC=CC=CC=CC(SCC(NC(=O)CCC(N)C(O)=O)C(=O)NCC(O)=O)C(O)CCCC(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=LEUKOTRIENE-C4

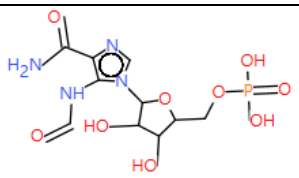
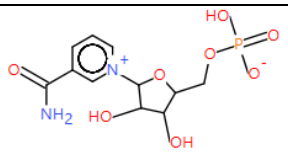
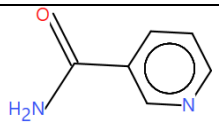
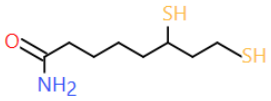
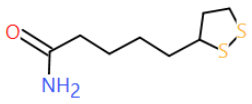
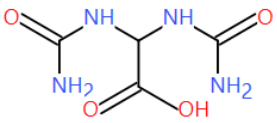
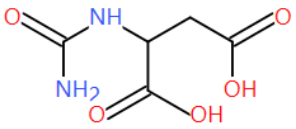
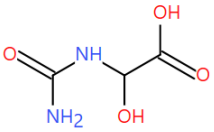
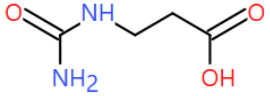
129	72059-45-1		CPD-8892	CCCCCC=CCC=CC=CC=CC1OC1CCCC(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD-8892
130	506-32-1	EC Number:2080334	ARACHIDONIC_ACID	CCCCCC=CCC=CCC=CCC=CCCCC(=O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=ARACHIDONIC_ACID
131			GAMMA-LINOLENOYL-COA	CCCCCC=CCC=CCC=CCCCCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc21		http://biocyc.org/HUMAN/NEW-IMAGE?object=GAMMA-LINOLENOYL-COA
132			CPD-18	CCCCCC=CCC=CCCCCCCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc21		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD-18
133			T2-DECENOYL-COA	CCCCCCCC=CC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12		http://biocyc.org/HUMAN/NEW-IMAGE?object=T2-DECENOYL-COA
134			OLEOYL-COA	CCCCCCCCC=CCCCCCCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n		http://biocyc.org/HUMAN/NEW-IMAGE?object=OLEOYL-COA

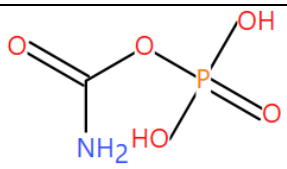
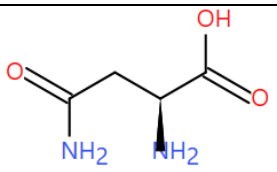
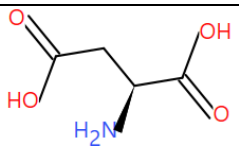
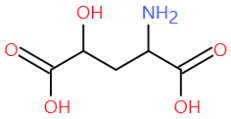
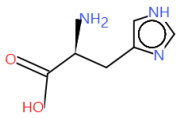
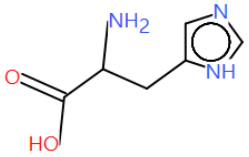
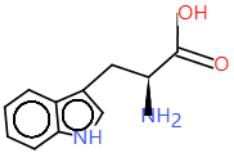
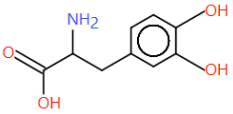
				1cnc2c(N)ncnc21		
135	112-80-1		OLEATE-CPD	CCCCCCCCC=CCCCCCCC(=O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=OLEATE-CPD
136			TETRADECANOYL-COA	CCCCCCCCCCCCCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12		http://biocyc.org/HUMAN/NEW-IMAGE?object=TETRADECANOYL-COA
137	362-66-3		STEAROYL-COA	CCCCCCCCCCCCCCCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12		http://biocyc.org/HUMAN/NEW-IMAGE?object=STEAROYL-COA
138	57-10-3	2003129	PALMITATE	CCCCCCCCCCCCCCCC(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=PALMITATE
139	1763-10-6		PALMITYL-COA	CCCCCCCCCCCCCCCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc21		http://biocyc.org/HUMAN/NEW-IMAGE?object=PALMITYL-COA
140	1118-68-9	2142678	DIMETHYL-GLYCINE	CN(C)CC(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=DIMETHYL-GLYCINE

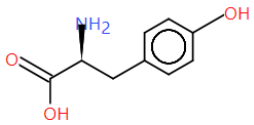
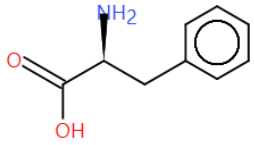
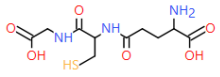
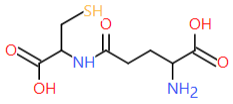
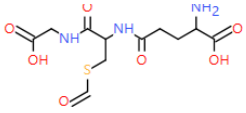
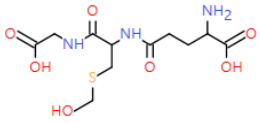
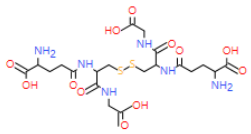
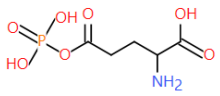
141	57-00-1	2003066	CREATINE	CN(CC(=O)O)C(=N)N		http://biocyc.org/HUMAN/NEW-IMAGE?object=CREATINE
142	67-07-2		CREATINE-P	CN(CC(=O)O)C(N)=NP(=O)(O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CREATINE-P
143	541-14-0		D-CARNITINE	C[N+](C)(C)CC(O)CC(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CARNITINE
144	7418-61-3		BETAINE_ALDEHYDE	C[N+](C)(C)CC=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=BETAINE_ALDEHYDE
145			3-HYDROXY-N6N6N6-TRIMETHYL-L-LYSINE	C[N+](C)(C)CCCC(O)C(N)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=3-HYDROXY-N6N6N6-TRIMETHYL-L-LYSINE
146			4-TRIMETHYLAMMONIOBUTANAL	C[N+](C)(C)CCCC=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=4-TRIMETHYLAMMONIOBUTANAL
147	123-41-1		CHOLINE	C[N+](C)(C)CCO		http://biocyc.org/HUMAN/NEW-IMAGE?object=CHOLINE
148			L-1-GLYCERO-PHOSPHORYLCHOLINE	C[N+](C)(C)CCOP(O)(=O)OCC(O)CO		http://biocyc.org/HUMAN/NEW-IMAGE?object=L-1-GLYCERO-PHOSPHORYLCHOLINE
149	107-73-3		PHOSPHORYL-CHOLINE	C[N+](C)(C)CCOP(O)(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=PHOSPHORYL-CHOLINE
150	107-43-7	2034906	BETAINE	C[N+](C)(C)CC(=O)[O-]		http://biocyc.org/HUMAN/NEW-IMAGE?object=BETAINE

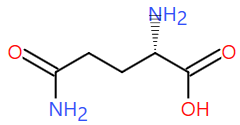
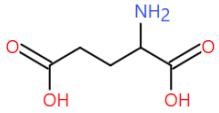
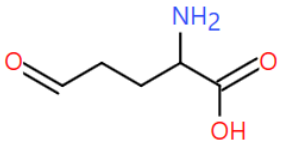
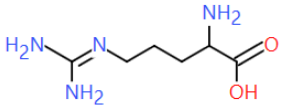
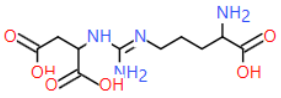
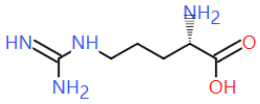
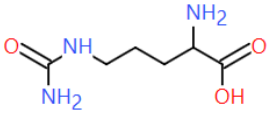
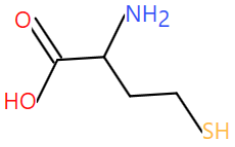
151		541-15-1	CARNITINE	C[N+](C)(C)CC(O)CC([O-])=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CARNITINE
152			N6N6N6-TRIMETHYL-L-LYSINE	[H]C(N)(CCCC[N+](C)(C)C)C(=O)[O-]		http://biocyc.org/HUMAN/NEW-IMAGE?object=N6N6N6-TRIMETHYL-L-LYSINE
153			CPD-396	C[n+]1cccc(c1)C(N)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD-396
154	134-35-0		5-METHYL-THF_2	CN1C(CNc2ccc(cc2)C(=O)N[C@@H](CCC(O)=O)C(O)=O)CNC2N=C(N)NC(=O)C1=2		http://biocyc.org/HUMAN/NEW-IMAGE?object=5-METHYL-THF
155	134-35-0		5-METHYL-THF	CN1C(CNc2ccc(cc2)C(=O)N[C@@H](CCC(O)=O)C(O)=O)CNC2N=C(N)NC(=O)C1=2		http://biocyc.org/HUMAN/NEW-IMAGE?object=5-METHYL-THF
156	107-97-1	2035386	SARCOSINE	CNCC(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=SARCOSINE
157			CPD-7650	COc1cc(CCN)ccc1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD-7650
158			S-ADENOSYLMETHIONINAMINE	C[S+](CCCN)CC1OC(C(O)C1O)n1cnc2c(N)ncnc21		http://biocyc.org/HUMAN/NEW-IMAGE?object=S-ADENOSYLMETHIONINAMINE

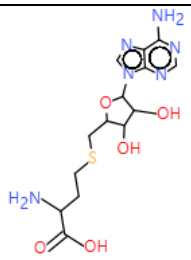
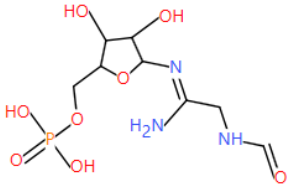
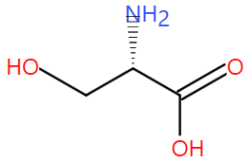
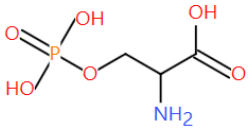
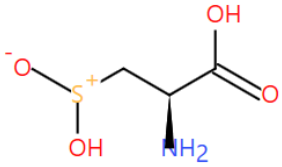
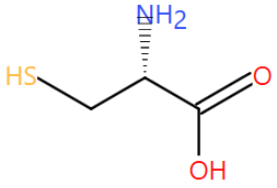
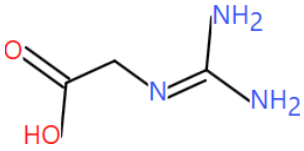
159	29908-03-0		S-ADENOSYLMETHIONINE	C[S+](CCC(N)C([O-])=O)CC1OC(C(O)C1O)n1cnc2c(N)ncnc21		http://biocyc.org/HUMAN/NEW-IMAGE?object=S-ADENOSYLMETHIONINE
160	2457-80-9		5-METHYLTHIOADENOSINE	CSCC1OC(C(O)C1O)n1cnc2c(N)ncnc21		http://biocyc.org/HUMAN/NEW-IMAGE?object=5-METHYLTHIOADENOSINE
161			CPD-444	CSCC1OC(OP(O)(O)=O)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD-444
162	63-68-3	2005629	METHIONINE	CSCC[C@H](N)C(O)=O		
163			IODINE-MOLECULE	II		http://biocyc.org/HUMAN/NEW-IMAGE?object=IODINE-MOLECULE
164	7664-41-7	2316353	AMMONIA	N		http://biocyc.org/HUMAN/NEW-IMAGE?object=AMMONIA
165			PHOSPHORIBOSYL-ATP	OC1C(COP(O)(O)=O)OC(C1O)N1C=Nc2c(ncn2C2OC(COP(O)(=O)OP(O)(=O)OP(O)(O)=O)C(O)C2O)C1=N		http://biocyc.org/HUMAN/NEW-IMAGE?object=PHOSPHORIBOSYL-ATP
166		2332710	NITRIC-OXIDE	N=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=NITRIC-OXIDE
167			2-AMINOMUCONATE_SEMIALDEHYDE	NC(=CC=CC=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=2-AMINOMUCONATE_SEMIALDE

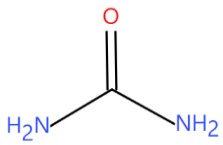
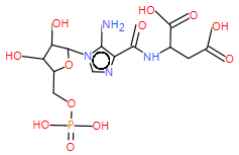
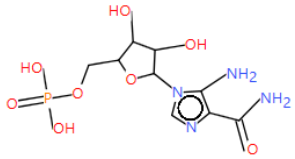
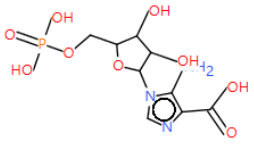
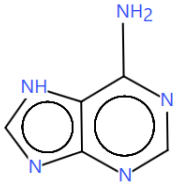
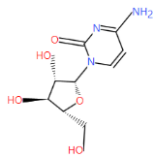
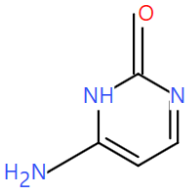
						HYDE
168			PHOSPHORIBOSYL-FORMAMIDO-CARBOXAMIDE	NC(=O)c1ncn(C2OC(COP(O)(O)=O)C(O)C2O)c1NC=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=PHOSPHORIBOSYL-FORMAMIDO-CARBOXAMIDE
169	1094-61-7		NICOTINAMIDE_NUCLEOTIDE	NC(=O)c1ccc[n+](c1)C1OC(COP(O)([O-])=O)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=NICOTINAMIDE_NUCLEOTIDE
170	98-92-0	2027134	NIACINAMIDE	NC(=O)c1cccnc1		http://biocyc.org/HUMAN/NEW-IMAGE?object=NIACINAMIDE
171			DIHYDROLIPOAMIDE	NC(=O)CCCCC(S)CCS		http://biocyc.org/HUMAN/NEW-IMAGE?object=DIHYDROLIPOAMIDE
172	940-69-2	2133752	LIPOAMIDE	NC(=O)CCCCC1CCSS1		http://biocyc.org/HUMAN/NEW-IMAGE?object=LIPOAMIDE
173	99-16-1	EC Number:2027354	ALLANTOATE	NC(=O)NC(NC(N)=O)C(=O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=ALLANTOATE
174	16649-79-9		CARBAMYUL-L-ASPARTATE	NC(=O)NC(CC(O)=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CARBAMYUL-L-ASPARTATE
175			CPD-1091	NC(=O)NC(O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD-1091
176			3-UREIDO-PROPIONATE	NC(=O)NCCC(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=3-UREIDO-PROPIONATE

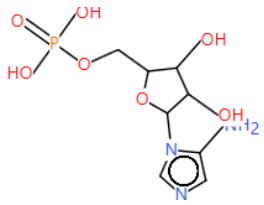
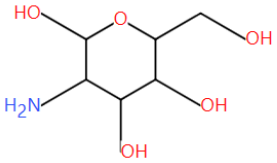
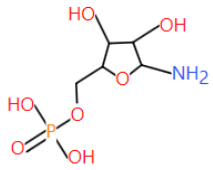
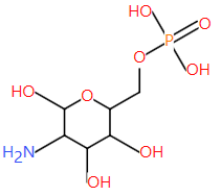
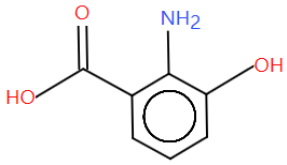
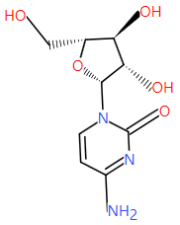
177	590-55-6		CARBAMOYL-P	NC(=O)OP(=O)(O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CARBAMOYL-P
178	70-47-3	2007359	ASPARAGINE	N[C@@H](CC(N)=O)C(O)=O		
179	56-84-8	2002916	L-ASPARTIC ACID	N[C@@H](CC(O)=O)C(O)=O		
180			L-ERYTHRO-4-HYDROXY-GLUTAMATE	NC(CC(O)C(O)=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=L-ERYTHRO-4-HYDROXY-GLUTAMATE
181	71-00-1		HISTIDINE	N[C@@H](CC1=CNC=N1)C(O)=O		
182	71-00-1		HIS	[H]C(N)(CC1=CN=CN1)C(=O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=HIS
183	73-22-3	2007956	TRYPTOPHAN	N[C@@H](Cc1c[nH]c2ccccc12)C(O)=O		
184	59-92-7		L-DIHYDROXY-PHENYLALANINE	[H]C(N)(CC=1C=CC(O)=C(O)C=1)C(=O)O		
185	60-18-4	2004604	TYROSINE	N[C@@H](Cc1ccc(O)cc1)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=L-

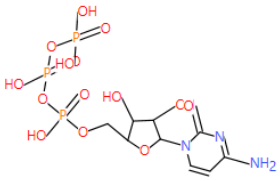
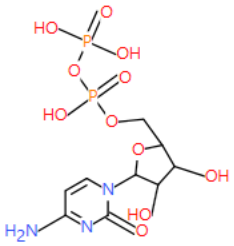
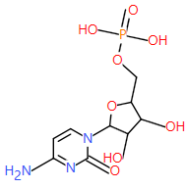
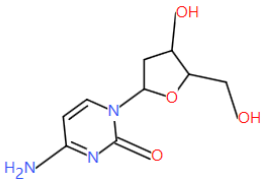
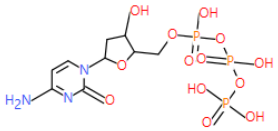
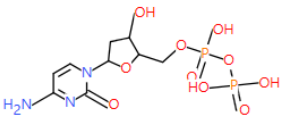
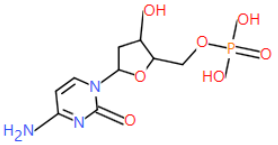
						DIHYDROXY-PHENYLALANINE
186	63-91-2	2005681	PHENYLALANINE	N[C@@H](Cc1ccccc1)C(O)=O		
187	70-18-8		GLUTATHIONE	NC(CCC(=O)NC(CS)C(=O)NCC(O)=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=GLUTATHIONE
188	686-58-8		L-GAMMA-GLUTAMYLCYSTEINE	NC(CCC(=O)NC(CS)C(O)=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=L-GAMMA-GLUTAMYLCYSTEINE
189			CPD-548	NC(CCC(=O)NC(CSC=O)C(=O)NCC(O)=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD-548
190			S-HYDROXYMETHYLGLUTATHIONE	NC(CCC(=O)NC(CSCO)C(=O)NCC(O)=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=S-HYDROXYMETHYLGLUTATHIONE
191	27025-41-8		OXIDIZED-GLUTATHIONE	NC(CCC(=O)NC(CSSCC(NC(=O)CCC(N)C(O)=O)C(=O)NCC(O)=O)C(=O)NCC(O)=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=OXIDIZED-GLUTATHIONE
192			L-GLUTAMATE-5-P	NC(CCC(=O)OP(O)(O)=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=L-GLUTAMATE-5-P
193	56-85-9	2002921	GLUTAMINE	N[C@@H](CCC(N)=O)C(O		

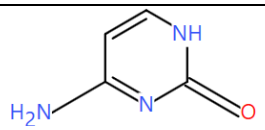
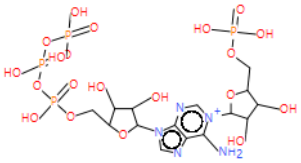
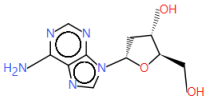
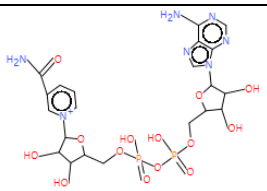
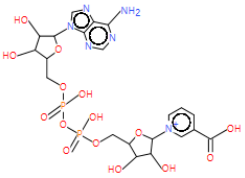
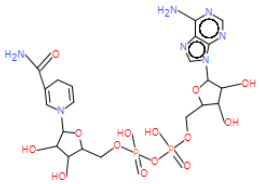
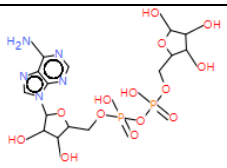
				)=O		
194	56-86-0	2002937	L-GLUTAMIC ACID	NC(CCC(O)=O)C(O)=O		
195			L-GLUTAMATE_GAMMA-SEMIALDEHYDE	NC(CCC=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=L-GLUTAMATE_GAMMA-SEMIALDEHYDE
196	74-79-3		ARG	NC(CCCN=C(N)N)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=ARG
197			L-ARGININO-SUCCINATE	NC(CCCN=C(N)NC(CC(O)=O)C(O)=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=L-ARGININO-SUCCINATE
198	74-79-3		L-ARGININE	N[C@@H](CCCNC(N)=N)C(O)=O		
199	372-75-8	2067596	L-CITRULLINE	NC(CCCNC(N)=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=L-CITRULLINE
200	454-28-4		HOMO-CYS	NC(CCS)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=HOMO-CYS
201	979-92-0		ADENOSYL-HOMO-CYS	NC(CCSCC1OC(C(O)C1O)n1cnc2c(N)ncnc21)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=ADENOSYL-HOMO-CYS

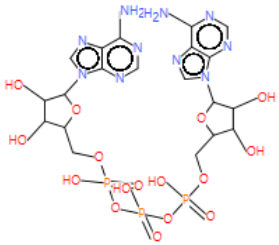
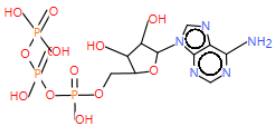
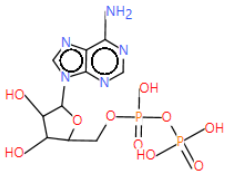
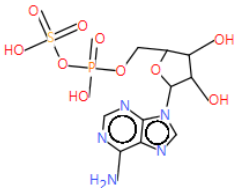
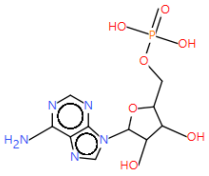
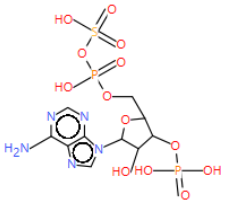
						
202			5-PHOSPHORIBOSYL-N-FORMYLGLYCINEAMIDINE	NC(CNC=O)=NC1OC(COP(O)(O)=O)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=5-PHOSPHORIBOSYL-N-FORMYLGLYCINEAMIDINE
203	56-45-1	2002743	SERINE	N[C@@H](CO)C(O)=O		
204	17885-08-4		3-P-SERINE	NC(COP(O)(O)=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=3-P-SERINE
205	1115-65-7	2142285	3-SULFINOALANINE	N[C@@H](C[S+](O)[O-])C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=3-SULFINOALANINE
206	52-90-4	2001582	CYSTEINE	N[C@@H](CS)C(O)=O		
207	352-97-6	2065295	GUANIDOACETIC_ACID	NC(N)=NCC(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=GUANIDOACETIC_ACID

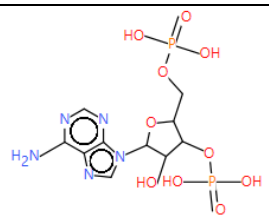
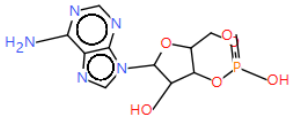
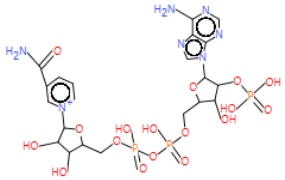
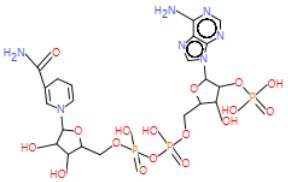
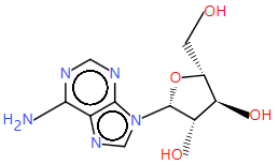
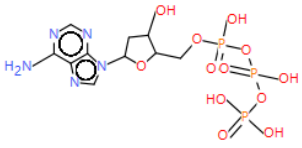
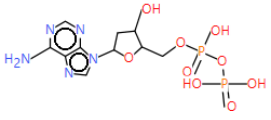
208	57-13-6		UREA	NC(N)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=UREA
209			P-RIBOSYL-4-SUCCCARB-AMINOIMIDAZOLE	Nc1c(ncn1C1OC(COP(O)(O)=O)C(O)C1O)C(=O)NC(CC(O)=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=P-RIBOSYL-4-SUCCCARB-AMINOIMIDAZOLE
210	3031-94-5		AICAR	NC(=O)c1ncn(C2OC(COP(O)(O)=O)C(O)C2O)c1N		http://biocyc.org/HUMAN/NEW-IMAGE?object=AICAR
211			PHOSPHORIBOSYL-CARBOXY-AMINOIMIDAZOLE	Nc1c(ncn1C1OC(COP(O)(O)=O)C(O)C1O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=PHOSPHORIBOSYL-CARBOXY-AMINOIMIDAZOLE
212	73-24-5		ADENINE_2	Nc1ncnc2nc[nH]c12		http://biocyc.org/HUMAN/NEW-IMAGE?object=ADENINE
213	65-46-3	2006109	CYTIDINE	NC1C=CN([C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O)C(=O)N=1		
214	71-30-7		CCYTOSINE_2	NC1NC(=O)N=CC=1		http://biocyc.org/HUMAN/NEW-IMAGE?object=CYTOSINE
215	25635-88-5		5-PHOSPHORIBOSYL-5-AMINOIMIDA	Nc1cncn1C1OC(COP(O)(O)=O)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=5-PHOSPHORIBOS

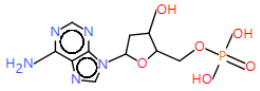
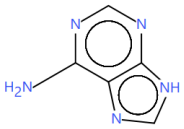
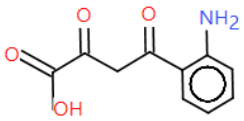
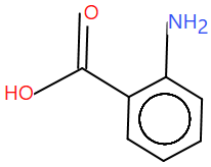
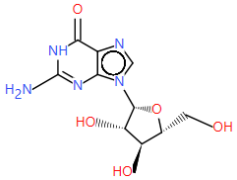
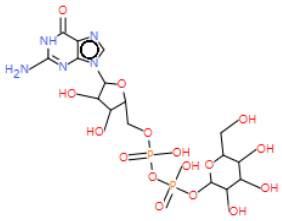
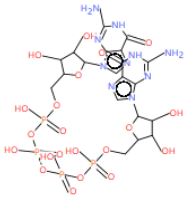
			ZOLE			YL-5-AMINOIMIDAZOLE
216	3416-24-8		GLUCOSAMINE	NC1C(O)OC(CO)C(O)C1O		
217			5-P-BETA-D-RIBOSYL-AMINE	NC1OC(COP(O)(O)=O)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=5-P-BETA-D-RIBOSYL-AMINE
218	3616-42-0		D-GLUCOSAMINE-6-P	NC1C(O)OC(COP(O)(O)=O)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=D-GLUCOSAMINE-6-P
219	548-93-6	2089625	3-HYDROXY-ANTHRANILATE	Nc1c(O)cccc1C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=3-HYDROXY-ANTHRANILATE
220	65-46-3	2006109	CYTIDINE_2	NC1C=CN([C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O)C(=O)N=1		http://biocyc.org/HUMAN/NEW-IMAGE?object=CYTIDINE
221			Cytidine triphosphate	NC1C=CN(C2OC(COP(O)(=O)OP(O)(=O)OP(O)(O)=O)		

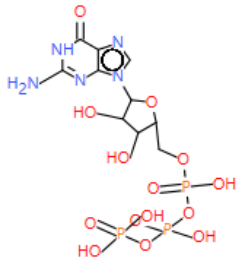
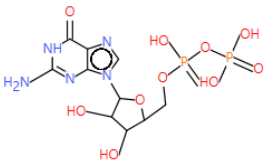
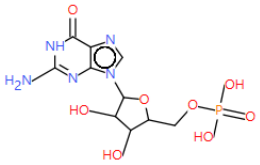
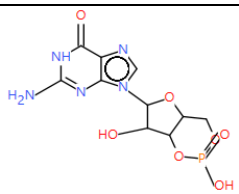
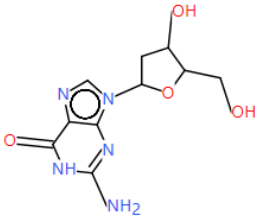
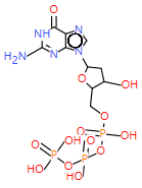
				C(O)C2O)C(=O)N=1		
222			Cytidine diphosphate	NC=1C=CN(C(=O)N=1)C2OC(COP(O)(=O)OP(O)(O)=O)C(O)C2(O)		
223			Cytidine monophosphate	NC1C=CN(C2OC(COP(O)(O)=O)C(O)C2O)C(=O)N=1		
224	951-77-9		DEOXYCYTIDINE	NC1C=CN(C2CC(O)C(CO)O2)C(=O)N=1		
225			Deoxycytidine triphosphate	NC=1C=CN(C(=O)N=1)C2CC(O)C(COP(=O)(O)OP(=O)(O)OP(=O)(O)O)O2		
226			Deoxycytidine diphosphate	NC1C=CN(C2CC(O)C(COP(O)(=O)OP(O)(O)=O)O2)C(=O)N=1		
227			Deoxycytidine monophosphate	NC=1C=CN(C(=O)N=1)C2CC(O)C(COP(O)(O)=O)O2		

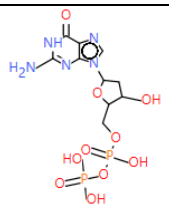
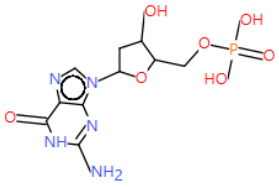
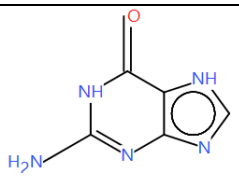
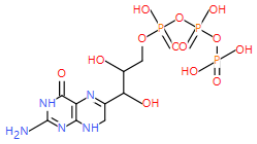
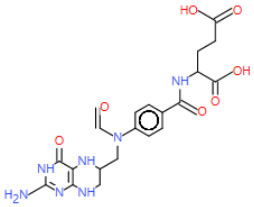
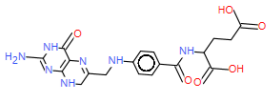
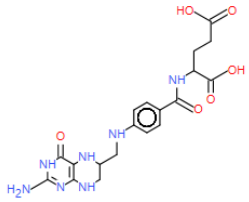
228	71-30-7	2007495	CYTOSINE	NC1=NC(=O)NC=C1		
229			PHOSPHORIBOSYL-ATP_1	Nc1c2ncn(C3OC(COP(O)(=O)OP(O)(=O)OP(O)(O)=O)C(O)C3O)c2nc[n+]1C1OC(COP(O)(O)=O)C(O)C1O		
230	958-09-8	2134887	DEOXYADENOSINE	Nc1ncnc2c1ncn2[C@@H]1C[C@H](O)[C@@H](CO)O1		**Error! Not a valid link.**
231	53-84-9		NADH	NC(=O)c1ccc[n+](c1)C1OC(COP(O)(=O)OP(O)(=O)OCC2OC(C(O)C2O)n2cnc3c(N)ncnc23)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=NADH
232	6450-77-7		DEAMIDO-NAD	Nc1ncnc2c1ncn2C1OC(COP(O)(=O)OP(O)(=O)OCC2OC(C(O)C2O)[n+]2cccc(c2)C(O)=O)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=DEAMIDO-NAD
233	53-84-9		NADH	NC(=O)C1CC=CN(C=1)C1OC(COP(O)(=O)OP(O)(=O)OCC2OC(C(O)C2O)n2cnc3c(N)ncnc32)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=NAD
234	20762-30-5		ADENOSINE_DIPHOSPHATE_RIBOSE	Nc1ncnc2c1ncn2C1OC(COP(O)(=O)OP(O)(=O)OCC2OC(O)C(O)C2O)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=ADENOSINE_DIPHOSPHATE_RIBOSE

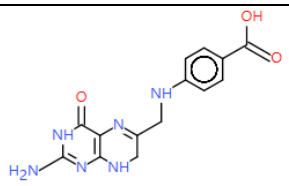
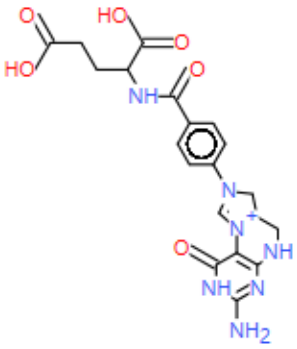
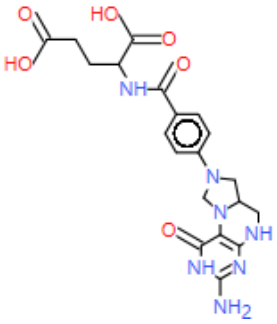
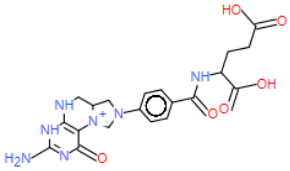
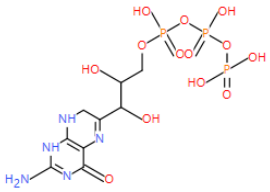
235			ADENOSINE5TRIPHOSPHO5ADENOSINE	Nc1ncnc2c1ncn2C1OC(COP(O)(=O)OP(O)(=O)OP(O)(=O)OCC2OC(C(O)C2O)n2cnc3c(N)ncnc32)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=ADENOSINE5TRIPHOSPHO5ADENOSINE
236			Adenosine triphosphate	Nc1ncnc2c1ncn2C1OC(COP(O)(=O)OP(O)(=O)OP(O)(O)=O)C(O)C1O		
237			Adenosine diphosphate	Nc1ncnc2c1ncn2C1OC(COP(O)(=O)OP(O)(O)=O)C(O)C1O		
238	485-84-7		APS	Nc1ncnc2c1ncn2C1OC(COP(O)(=O)OS(O)(=O)=O)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=APS
239			Adenosine phosphate	NC3N=CN=C1C=3(N=CN1C2OC(COP(O)(O)=O)C(O)C2(O))		
240	482-67-7		PAPS	Nc1ncnc2c1ncn2C1OC(COP(O)(=O)OS(O)(=O)=O)C(OP(O)(O)=O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=PAPS
241	60-92-4		PAP	Nc1ncnc2c1ncn2C1OC(COP(O)(O)=O)C(OP(O)(O)=O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=PAP

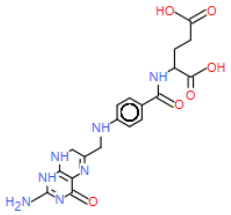
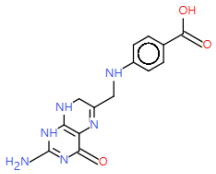
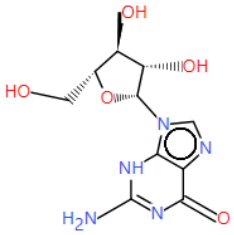
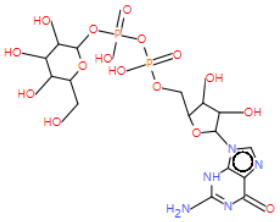
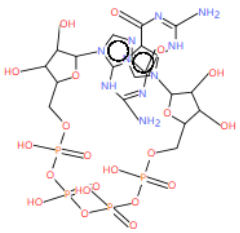
						
242	60-92-4		CAMP	Nc1ncnc2c1ncn2C1OC2COP(O)(=O)OC2C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CAMP
243	53-59-8		NADP	NC(=O)c1ccc[n+](c1)C1OC(COP(O)(=O)OP(O)(=O)OCC2OC(C(OP(O)(O)=O)C2O)n2cnc3c(N)ncnc32)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=NADP
244	2646-71-1		NADPH	NC(=O)C1CC=CN(C=1)C1OC(COP(O)(=O)OP(O)(=O)OCC2OC(C(OP(O)(O)=O)C2O)n2cnc3c(N)ncnc23)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=NADPH
245	58-61-7	2003899	ADENOSINE	NC1=NC=NC2=C1N=CN2[C@@H]3O[C@H](CO)[C@@H](O)[C@H]3O		
246			Deoxyadenosine triphosphate	Nc1ncnc2c1ncn2C1CC(O)C(COP(O)(=O)OP(O)(=O)OP(O)(O)=O)O1		
247			Deoxyadenosine diphosphate	NC3=NC=NC2=C3(N=CN2(C1CC(O)C(COP(=O)(O)OP(=O)(O)O)O1))		

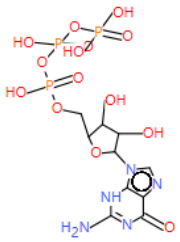
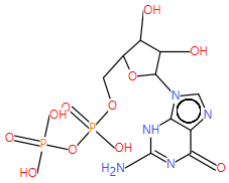
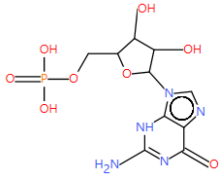
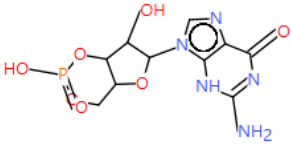
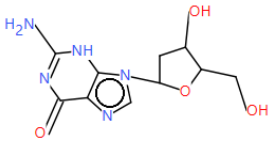
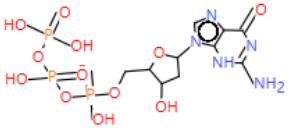
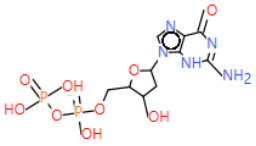
248			Deoxyadenosine monophosphate	NC3=NC=NC2=C3(N=CN2(C1CC(O)C(COP(O)(O)=O)O1))		
249	73-24-5	2007961	ADENINE	NC1C2NC=NC=2N=CN=1		
250			CPD-476	Nc1ccccc1C(=O)CC(=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD-476
251	118-92-3	2042875	ANTHRANILATE	NC1=CC=CC=C1(C(=O)O)		http://biocyc.org/HUMAN/NEW-IMAGE?object=ANTHRANILATE
252	118-00-3		GUANOSINE_2	NC1NC(=O)c2ncn([C@@H]3O[C@H](CO)[C@@H](O)[C@H]3O)c2N=1		http://biocyc.org/HUMAN/NEW-IMAGE?object=GUANOSINE
253			GDP-MANNOSE_1	NC1NC(=O)c2ncn(C3OC(COP(O)(=O)OP(O)(=O)OC4OC(CO)C(O)C(O)C4O)C(O)C3O)c2N=1		http://biocyc.org/HUMAN/NEW-IMAGE?object=GDP-MANNOSE_1
254			CPD-609	NC1NC(=O)c2ncn(C3OC(COP(O)(=O)OP(O)(=O)OP(O)(=O)OP(O)(=O)OCC4OC(C(O)C4O)n4cnc5C(=O)NC(N)=Nc54)C(O)C3O)c2N=1		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD-609
255			Guanosine triphosphate	NC1NC(=O)c2ncn(C3OC(COP(O)(=O)OP(		

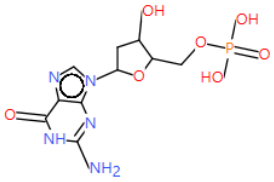
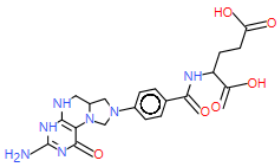
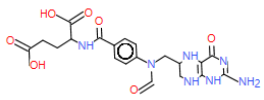
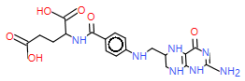
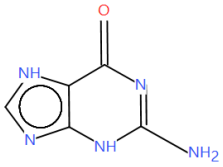
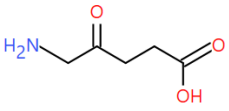
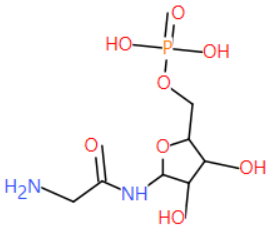
				O)(=O)OP(O)(O)=O)C(O)C3O)c2N=1		
256			Guanosine diphosphate	NC1NC(=O)c2ncn(C3OC(COP(O)(=O)OP(O)(O)=O)C(O)C3O)c2N=1		
257			Guanosine monophosphate	NC1NC(=O)C=2N=CN(C=2(N=1))C3OC(COP(O)(O)=O)C(O)C3(O)		
258	7665-99-8		CGMP	NC1NC(=O)c2ncn(C3OC4COP(O)(=O)OC4C3O)c2N=1		http://biocyc.org/HUMAN/NEW-IMAGE?object=CGMP
259	961-07-9		DEOXYGUANOSINE	NC1NC(=O)c2ncn(C3CC(O)C(CO)O3)c2N=1		http://biocyc.org/HUMAN/NEW-IMAGE?object=DEOXYGUANOSINE
260			Deoxyguanosine triphosphate	NC1NC(=O)c2ncn(C3CC(O)C(COP(O)(=O)OP(O)(=O)OP(O)(O)=O)O3)c2N=1		

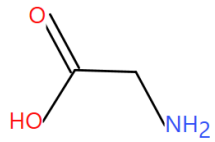
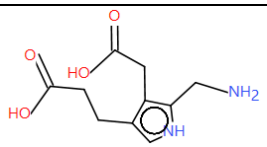
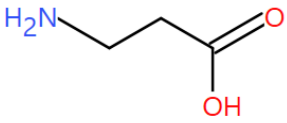
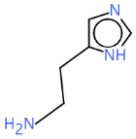
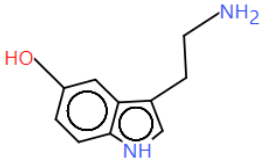
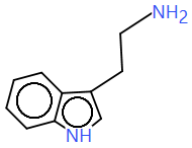
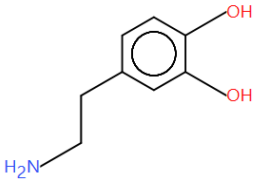
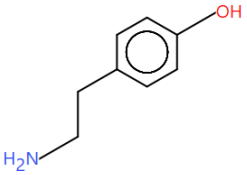
261			Deoxyguanosine diphosphate_2	NC1NC(=O)c2ncn(C3CC(O)C(COP(O)(=O)OP(O)(O)=O)O3)c2N=1		http://biocyc.org/HUMAN/NEW-IMAGE?object=Deoxyguanosine diphosphate
262			Deoxyguanosine monophosphate_2	NC1NC(=O)c2ncn(C3CC(O)C(COP(O)(O)=O)O3)c2N=1		http://biocyc.org/HUMAN/NEW-IMAGE?object=Deoxyguanosine monophosphate
263	73-40-5		GUANINE	NC1=NC2=C(NC=N2)C(=O)N1		
264			DIHYDRONEOPTERIN-P3	NC1NC(=O)C2N=C(CNC=2N=1)C(O)C(O)COP(O)(=O)OP(O)(=O)OP(O)(O)=O		
265	2800-34-2		10-FORMYL-THF_2	NC1NC(=O)C2NC(CNC=2N=1)CN(C=O)c1ccc(cc1)C(=O)NC(CCC(O)=O)C(O)=O		
266	4033-27-6		DIHYDROFOLATE_2	NC1NC(=O)C2N=C(CNc3ccc(cc3)C(=O)NC(CCC(O)=O)C(O)=O)CNC=2N=1		http://biocyc.org/HUMAN/NEW-IMAGE?object=DIHYDROFOLATE
267	29347-89-5		THF	NC1NC(=O)C2NC(CNc3ccc(cc3)C(=O)NC(CCC(O)=O)C(O)=O)CNC=2N=1		http://biocyc.org/HUMAN/NEW-IMAGE?object=THF
268			7-8-DIHYDROPTEROATE	NC1NC(=O)C2N=C(CNc3ccc(cc3)C(O)=O)CNC=2N=1		http://biocyc.org/HUMAN/NEW-IMAGE?object=7-8-

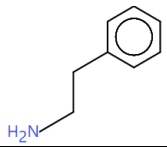
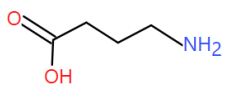
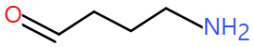
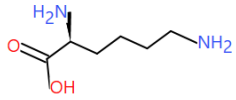
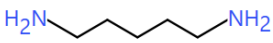
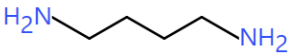
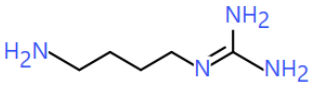
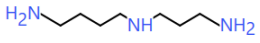
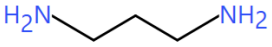
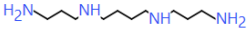
						DIHYDROPTEROATE
269	7444-29-3		5-10-METHENYL-THF	NC1NC(=O)C2=C(NCC3CN(C=[N+]32)c2ccc(cc2)C(=O)NC(CCC(O)=O)C(O)=O)N=1		http://biocyc.org/HUMAN/NEW-IMAGE?object=5-10-METHENYL-THF
270			METHYLENE-THF	NC1NC(=O)C2N3CN(CC3CNC=2N=1)c1ccc(cc1)C(=O)NC(CCC(O)=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=METHYLENE-THF
271	7444-29-3		5-10-METHENYL-THF_2	NC1NC2NCC3CN(C=[N+]3C=2C(=O)N=1)c1ccc(cc1)C(=O)NC(CCC(O)=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=5-10-METHENYL-THF
272			DIHYDRONEOPTERIN-P3_2	NC1NC2NCC(=NC=2C(=O)N=1)C(O)C(O)COP(O)(=O)OP(O)(=O)OP(O)(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=DIHYDRONEOPTERIN-P3

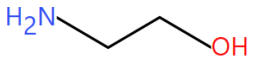
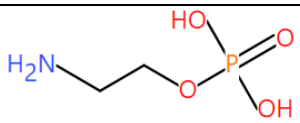
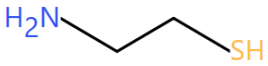
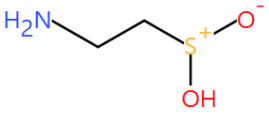
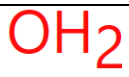
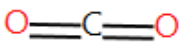
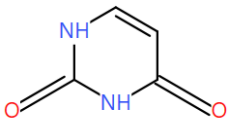
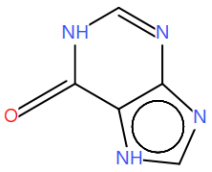
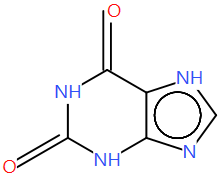
273	4033-27-6		DIHYDROFOLATE	[H]C(CCC(=O)O)(NC(=O)C1=CC=C(C=C1)NCC=2CNC=3N=C(N)NC(=O)C=3(N=2))C(=O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=DIHYDROFOLATE
274			7-8-DIHYDROPTEROATE_2	NC2=NC(=O)C=3N=C(CNC1=CC=C(C=C1)C(=O)O)CNC=3(N2)		http://biocyc.org/HUMAN/NEW-IMAGE?object=7-8-DIHYDROPTEROATE
275	118-00-3		GUANOSINE	NC1=NC2=C(N=CN2[C@@H]3O[C@H](CO)[C@@H](O)[C@H]3O)C(=O)N1		
276			GDP-MANNOSE_2	NC1Nc2c(ncn2C2OC(COP(O)(=O)OP(O)(=O)OC3OC(CO)C(O)C(O)C3O)C(O)C2O)C(=O)N=1		http://biocyc.org/HUMAN/NEW-IMAGE?object=GDP-MANNOSE
277			CPD-609_2	NC1Nc2c(ncn2C2OC(COP(O)(=O)OP(O)(=O)OP(O)(=O)OP(O)(=O)OCC3OC(C(O)C3O)n3cnc4C(=O)N=C(N)Nc34)C(O)C2O)C(=O)N=1		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD-609
278			Guanosine triphosphate_2	NC1Nc2c(ncn2C2OC(COP(O)(=O)OP(O)(=O)OP(O)(O)=O)C(O)C2O)C(=O)N=1		http://biocyc.org/HUMAN/NEW-IMAGE?object=Guanosine triphosphate

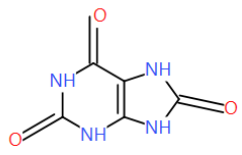
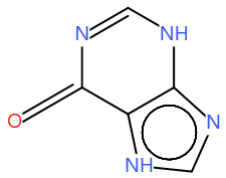
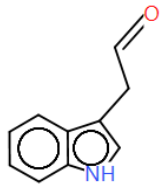
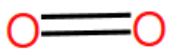
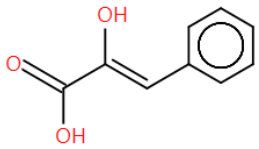
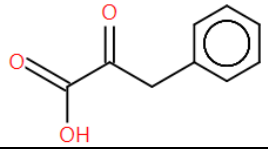
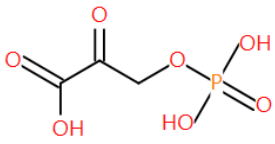
						
279				NC1Nc2c(ncn2C2OC(COP(O)(=O)OP(O)(O)=O)C(O)C2O)C(=O)N=1		http://biocyc.org/HUMAN/NEW-IMAGE?object=Guanosine diphosphate
280			Guanosine monophosphate_2	NC1Nc2c(ncn2C2OC(COP(O)(O)=O)C(O)C2O)C(=O)N=1		http://biocyc.org/HUMAN/NEW-IMAGE?object=Guanosine monophosphate
281	7665-99-8		961-07-9	NC1Nc2c(ncn2C2OC3COP(O)(=O)OC3C2O)C(=O)N=1		http://biocyc.org/HUMAN/NEW-IMAGE?object=GUANOSINE
282	961-07-9		DEOXYGUANOSINE_2	NC1Nc2c(ncn2C2CC(O)C(CO)O2)C(=O)N=1		http://biocyc.org/HUMAN/NEW-IMAGE?object=DEOXYGUANOSINE
283			Deoxyguanosine triphosphate_2	NC2=NC(=O)C=3N=CN(C1CC(O)C(COP(=O)(O)OP(=O)(O)OP(O)(=O)O)O1)C=3(N2)		http://biocyc.org/HUMAN/NEW-IMAGE?object=Deoxyguanosine triphosphate
284			Deoxyguanosine diphosphate	NC2NC(=O)C=3N=CN(C1CC(O)C(COP(=O)(O)OP(=O)(O)O)O1)C=3(N=2)		

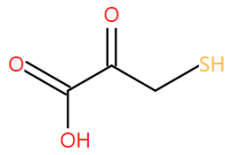
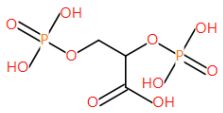
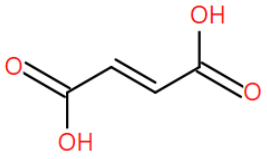
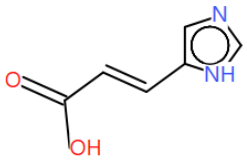
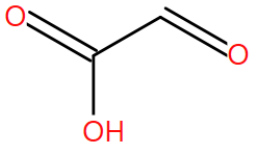
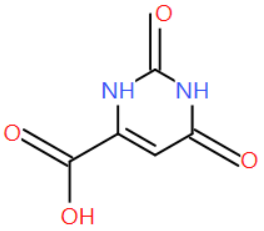
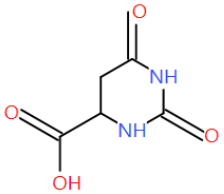
285			Deoxyguanosine monophosphate	NC2NC(=O)C=3N=CN(C1CC(O)C(COP(=O)(O)O)O1)C=3(N=2)		
286			METHYLENE-THF_2	[H]C24(CNC=1NC(N)=NC(=O)C=1N4(CN(C2)C3=CC=C(C=C3)C(=O)NC(CCC(=O)O)C(=O)O))		
287			10-FORMYL-THF	NC1NC(=O)C=2NC(CNC=2(N=1))CN(C=O)C3=CC=C(C=C3)C(=O)NC(CCC(=O)O)C(=O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=10-FORMYL-THF
288	29347-89-5		THF_2	NC2=NC(=O)C=3NC(CNC1=CC=C(C=C1)C(=O)NC(CCC(=O)O)C(=O)O)CNC=3(N2)		http://biocyc.org/HUMAN/NEW-IMAGE?object=THF
289	73-40-5		GUANINE_2	NC1NC2=C(NC=N2)C(=O)N=1		http://biocyc.org/HUMAN/NEW-IMAGE?object=GUANINE
290	106-60-5	2034141	5-AMINO-LEVULINATE	NCC(=O)CCC(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=5-AMINO-LEVULINATE
291			5-PHOSPHO-RIBOSYL-GLYCINEAMIDE	NCC(=O)NC1OC(COP(O)(O)=O)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=5-PHOSPHO-RIBOSYL-GLYCINEAMIDE

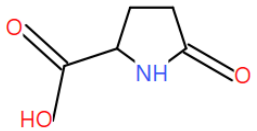
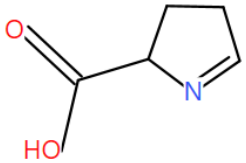
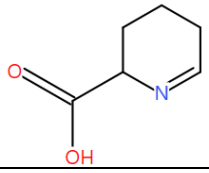
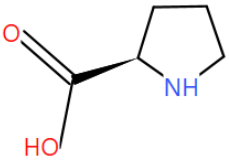
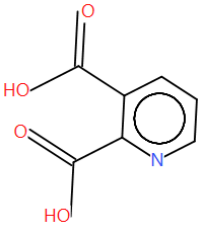
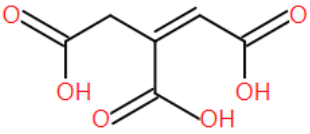
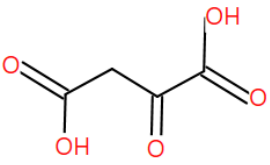
292	56-40-6	2002722	GLYCINE	NCC(O)=O		
293	487-90-1		PORPHOBILINOGEN	NCC=1NC=C(CCC(=O)O)C=1(CC(=O)O)		http://biocyc.org/HUMAN/NEW-IMAGE?object=PORPHOBILINOGEN
294	107-95-9		B-ALANINE	NCCC(=O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=B-ALANINE
295	51-45-6		HISTAMINE	NCCC1=CN=CN1		http://biocyc.org/HUMAN/NEW-IMAGE?object=HISTAMINE
296	50-67-9	2000589	SEROTONIN	NCCc1c[nH]c2ccc(O)cc12		http://biocyc.org/HUMAN/NEW-IMAGE?object=SEROTONIN
297	61-54-1	2005105	TRYPTAMINE	NCCc1c[nH]c2ccccc12		http://biocyc.org/HUMAN/NEW-IMAGE?object=TRYPTAMINE
298	51-61-6	2001100	DOPAMINE	NCCc1ccc(O)c(O)c1		http://biocyc.org/HUMAN/NEW-IMAGE?object=DOPAMINE
299	51-67-2	2001158	TYRAMINE	NCCc1ccc(O)cc1		http://biocyc.org/HUMAN/NEW-IMAGE?object=TYRAMINE

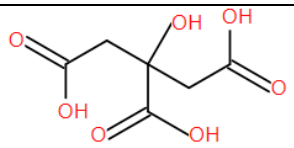
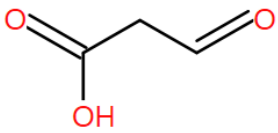
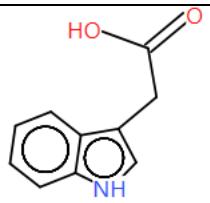
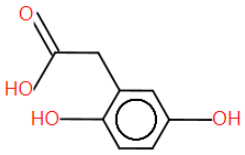
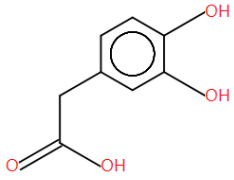
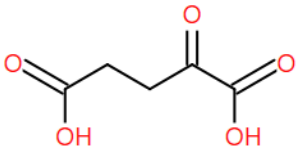
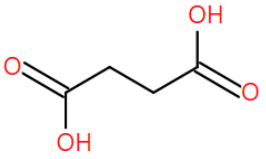
300	64-04-0	2005744	PHENYLETHYLAMINE	NCCC1=CC=CC=C1		http://biocyc.org/HUMAN/NEW-IMAGE?object=PHENYLETHYLAMINE
301	56-12-2	2002586	4-AMINO-BUTYRATE	NCCCC(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=4-AMINO-BUTYRATE
302	4390-05-0		4-AMINO-BUTYRALDEHYDE	NCCCC=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=4-AMINO-BUTYRALDEHYDE
303	56-87-1	2002942	LYSINE	NCCCC[C@H](N)C(O)=O		
304	462-94-2	2073290	CADAVERINE	NCCCCCN		http://biocyc.org/HUMAN/NEW-IMAGE?object=CADAVERINE
305	110-60-1	2037823	PUTRESCINE	NCCCCN		http://biocyc.org/HUMAN/NEW-IMAGE?object=PUTRESCINE
306	306-60-5	2061877	AGMATHINE	NCCCCN=C(N)N		http://biocyc.org/HUMAN/NEW-IMAGE?object=AGMATHINE
307	124-20-9	2046890	SPERMIDINE	NCCCCNCCCN		http://biocyc.org/HUMAN/NEW-IMAGE?object=SPERMIDINE
308	109-76-2	2037027	CPD-313	NCCCN		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD-313
309	71-44-3	2007542	SPERMINE	NCCCNCCCCNCCCN		http://biocyc.org/HUMAN/NEW-IMAGE?object=SPERMINE
310	141-43-5	2054833	ETHANOL-AMINE	NCCO		http://biocyc.org/HUMAN/NEW-

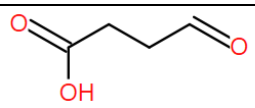
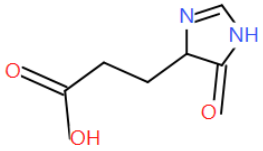
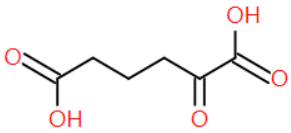
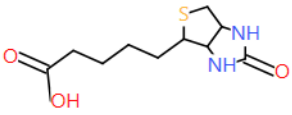
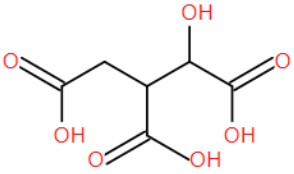
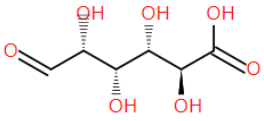
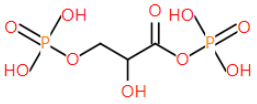
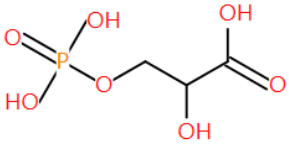
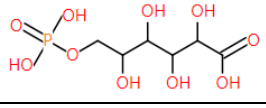
						IMAGE?object=ETHANOL-AMINE
311	1071-23-4	2139885	PHOSPHORYL-ETHANOLAMINE	NCCOP(O)(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=PHOSPHORYL-ETHANOLAMINE
312	60-23-1	2004630	CPD-239	NCCS		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD-239
313	300-84-5		HYPOTAURINE	NCC[S+](O)[O-]		http://biocyc.org/HUMAN/NEW-IMAGE?object=HYPOTAURINE
314	7732-18-5	2317912	Water	[OH2]		
315	124-38-9		CARBON-DIOXIDE	O=C=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CARBON-DIOXIDE
316	66-22-8	2006219	URACIL	O=C1NC=CC(=O)N1		
317	68-94-0	2006973	HYPOXANTHINE	O=C1NC=NC=2N=CNC1=2		http://biocyc.org/HUMAN/NEW-IMAGE?object=HYPOXANTHINE
318	69-89-6	2007186	XANTHINE	O=C1NC(=O)c2[nH]cnc2N1		http://biocyc.org/HUMAN/NEW-IMAGE?object=XANTHINE
319	69-93-2	2007207	URATE	O=C1NC(=O)C=2NC(=O)NC=2(N1)		http://biocyc.org/HUMAN/NEW-IMAGE?object=U

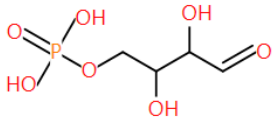
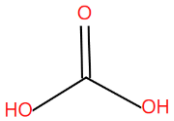
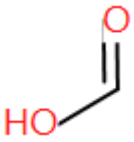
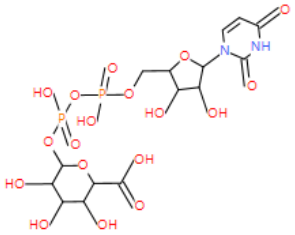
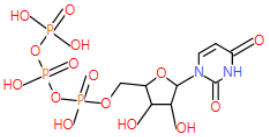
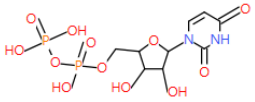
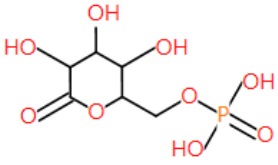
						RATE
320	68-94-0		HYPOXANTHINE_2	O=C1N=CNC=2N=CNC1=2		http://biocyc.org/HUMAN/NEW-IMAGE?object=HYPOXANTHINE
321	2591-98-2		INDOLE_ACETALDEHYDE	O=CCC1=CNC2=CC=CC=C12		http://biocyc.org/HUMAN/NEW-IMAGE?object=INDOLE_ACETALDEHYDE
322	7782-44-7		OXYGEN-MOLECULE	O=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=OXYGEN-MOLECULE
323	5801-57-0		ENOL-PHENYLPYRUVATE	O=C(O)C(O)=CC1=CC=CC=C1		http://biocyc.org/HUMAN/NEW-IMAGE?object=ENOL-PHENYLPYRUVATE
324	156-06-9	EC Number:2058471	PHENYL-PYRUVATE	O=C(O)C(=O)CC1=CC=CC=C1		http://biocyc.org/HUMAN/NEW-IMAGE?object=PHENYL-PYRUVATE
325	3913-50-6		3-P-HYDROXYPYRUVATE	O=C(O)C(=O)COP(=O)(O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=3-P-HYDROXYPYRUVATE
326	2464-23-5		3-MERCAPTO-PYRUVATE	OC(=O)C(=O)CS		http://biocyc.org/HUMAN/NEW-IMAGE?object=3-MERCAPTO-PYRUVATE

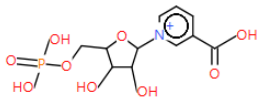
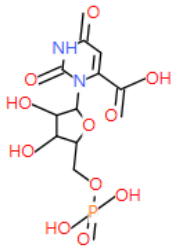
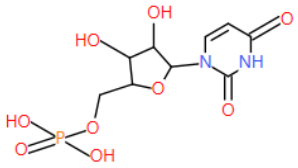
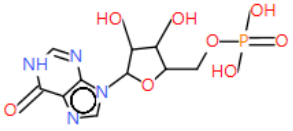
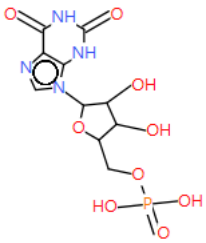
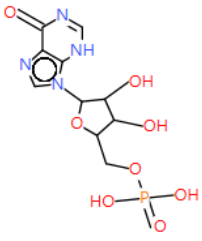
						
327			23-DIPHOSPHOGLYCERATE	OC(=O)C(COP(O)(O)=O)OP(O)(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=23-DIPHOSPHOGLYCERATE
328	110-17-8		FUM	O=C(O)C=CC(=O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=FUM
329	104-98-3		UROCANATE	O=C(O)C=CC1=CN=CN1		http://biocyc.org/HUMAN/NEW-IMAGE?object=UROCANATE
330	298-12-4	2060585	GLYOX	OC(=O)C=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=GLYOX
331	65-86-1	2006198	OROTATE	O=C(O)C1=CC(=O)NC(=O)N1		http://biocyc.org/HUMAN/NEW-IMAGE?object=OROTATE
332	155-54-4		DI-H-OROTATE	OC(=O)C1CC(=O)NC(=O)N1		http://biocyc.org/HUMAN/NEW-IMAGE?object=DI-H-OROTATE
333	98-79-3	2027003	DI-H-OROTATE	OC(=O)C1CCC(=O)N1		http://biocyc.org/HUMAN/NEW-IMAGE?object=D

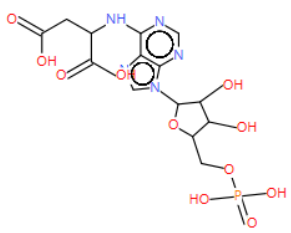
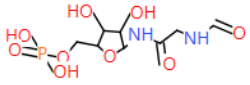
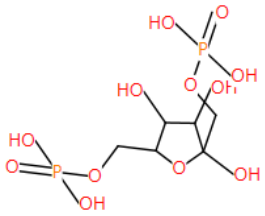
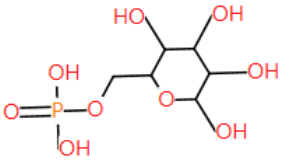
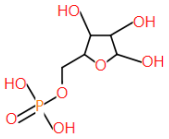
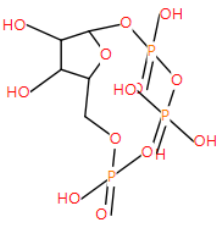
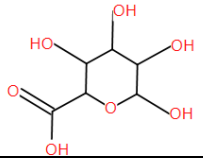
						I-H-OROTATE
334	2906-39-0		L-DELTA1-PYRROLINE_5-CARBOXYLATE	[H]C1(CCC=N1)C(=O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=L-DELTA1-PYRROLINE_5-CARBOXYLATE
335			CPD-7682	O=C(O)C1CCCC=N1		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD-7682
336	147-85-3		PROLINE	OC(=O)[C@H]1CCCN1		
337	89-00-9	2018748		OC(=O)c1ccccc1C(O)=O		
338	585-84-2		CIS-ACONITATE	O=C(O)C=C(CC(=O)O)C(=O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CIS-ACONITATE
339	328-42-7	2063298	CIS-ACONITATE	OC(=O)CC(=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CIS-ACONITATE

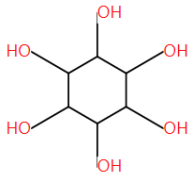
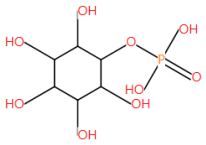
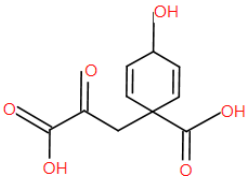
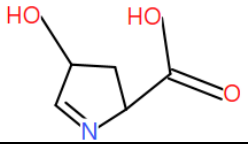
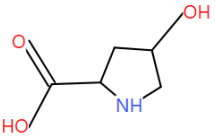
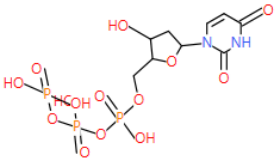
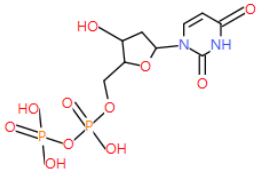
340	77-92-9	2010691	CIT	OC(=O)CC(O)(CC(O)=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CIT
341	926-61-4		MALONATE-S-ALD	OC(=O)CC=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=MALONATE-S-ALD
342	87-51-4	2017482	INDOLE_ACETATE_AUXIN	O=C(O)CC1=CNC2=CC=CC=C12		http://biocyc.org/HUMAN/NEW-IMAGE?object=INDOLE_ACETATE_AUXIN
343			HOMOGENTISATE	O=C(O)CC=1C=C(O)C=CC=1(O)		http://biocyc.org/HUMAN/NEW-IMAGE?object=HOMOGENTISATE
344	102-32-9	2030241	CPD-782	OC(=O)Cc1ccc(O)c(O)c1		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD-782
345	328-50-7	2063303	2-KETOGLUTARATE	O=C(O)CCC(=O)C(=O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=2-KETOGLUTARATE
346	110-15-6	2037404	SUC	O=C(O)CCC(=O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=SUC
347	692-29-5		SUCC-S-ALD	O=CCCC(=O)		http://biocyc.org/H

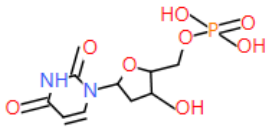
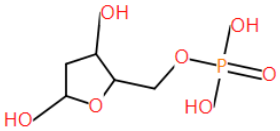
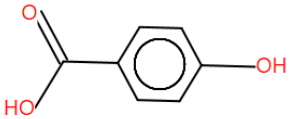
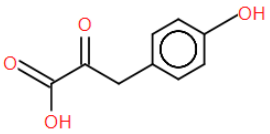
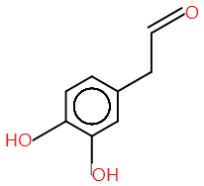
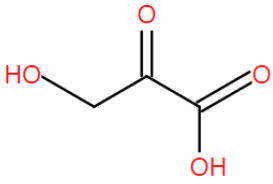
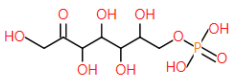
				O		UMAN/NEW-IMAGE?object=SUCC-S-ALD
348	17340-16-8		4-IMIDAZOLONE-5-PROPIONATE	OC(=O)CCC1N=CNC1=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=4-IMIDAZOLONE-5-PROPIONATE
349	3184-35-8		2K-ADIPATE	OC(=O)CCCC(=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=2K-ADIPATE
350	58-85-5		BIOTIN	OC(=O)CCCCC1SCC2NC(=O)NC21		http://biocyc.org/HUMAN/NEW-IMAGE?object=BIOTIN
351	320-77-4	2062823	THREO-DS-ISO-CITRATE	OC(C(CC(O)=O)C(O)=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=THREO-DS-ISO-CITRATE
352	576-37-4	2094017	GLUCURONIC ACID	O[C@@H](C=O)[C@@H](O)[C@H](O)[C@H](O)C(O)=O		
353	1981-49-3		DPG	[H]C(O)(COP(=O)(O)O)C(=O)OP(=O)(O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=DPG
354	820-11-1		G3P	OC(COP(O)(O)=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=G3P
355			CPD-2961	OC(COP(O)(O)=O)C(O)C(O)C(O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD-2961

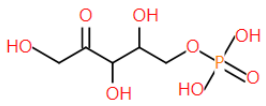
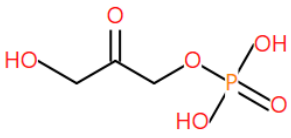
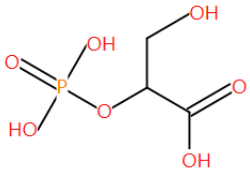
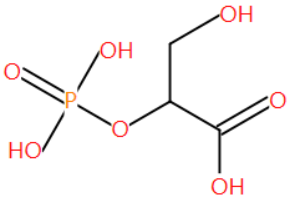
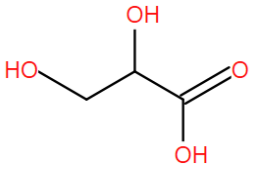
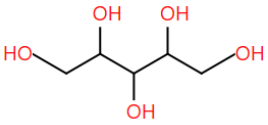
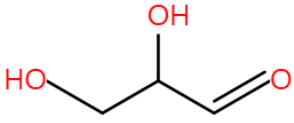
356	585-18-2		ERYTHROSE-4P	OC(COP(O)(O)=O)C(O)C=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=ERYTHROSE-4P
357	463-79-6		H2CO3	OC(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=H2CO3
358	64-18-6		FORMATE	OC=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=FORMATE
359	2616-64-0		UDP-GLUCURONATE	OC1C(COP(O)(=O)OP(O)(=O)OC2OC(C(O)C(O)C2O)C(O)=O)OC(C1O)N1C=CC(=O)NC1=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=UDP-GLUCURONATE
360			Uridine triphosphate	O=C1C=CN(C(=O)N1)C2OC(COP(O)(=O)OP(O)(=O)OP(O)(O)=O)C(O)C2(O)		
361			Uridine diphosphate	OC1C(COP(O)(=O)OP(O)(O)=O)OC(C1O)N1C=CC(=O)NC1=O		
362	2641-81-8		D-6-P-GLUCONO-DELTA-LACTONE	OC1C(O)C(COP(O)(O)=O)OC(=O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=D-6-P-GLUCONO-DELTA-LACTONE

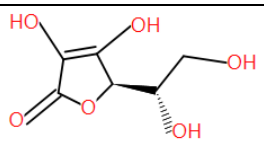
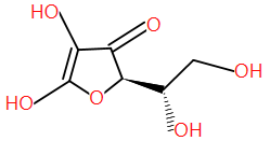
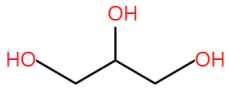
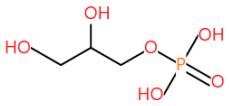
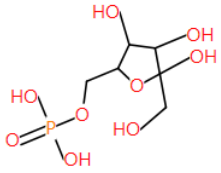
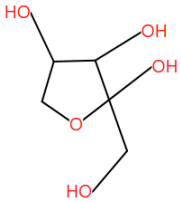
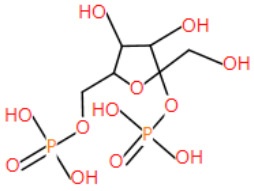
363	321-02-8		NICOTINATE_NUCLEOTIDE	OC1C(COP(O)(O)=O)OC(C1O)[n+]1cccc(c1)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=NICOTINATE_NUCLEOTIDE
364	2149-82-8		OROTIDINE-5-PHOSPHATE	OC1C(O)C(OC1COP(O)(O)=O)N1C(=O)NC(=O)C=C1C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=OROTIDINE-5-PHOSPHATE
365			Uridine monophosphate	O=C1C=CN(C(=O)N1)C2OC(COP(O)(O)=O)C(O)C2(O)		
366	131-99-7		IMP	OC1C(COP(O)(O)=O)OC(C1O)n1cnc2C(=O)NC=Nc21		http://biocyc.org/HUMAN/NEW-IMAGE?object=IMP
367			XANTHOSINE-5-PHOSPHATE	OC1C(COP(O)(O)=O)OC(C1O)n1cnc2C(=O)NC(=O)Nc21		http://biocyc.org/HUMAN/NEW-IMAGE?object=XANTHOSINE-5-PHOSPHATE
368	131-99-7		IMP_2	OC1C(COP(O)(O)=O)OC(C1O)n1cnc2C(=O)N=CNc21		http://biocyc.org/HUMAN/NEW-IMAGE?object=IMP
369	19240-42-7		ADENYLOSUCC	OC1C(COP(O)(O)=O)OC(C1O)n1cnc2c(NC(CC(O)=O)C		http://biocyc.org/HUMAN/NEW-IMAGE?object=ADENYLOSUCC

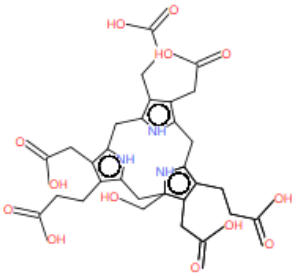
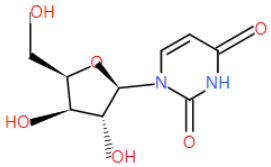
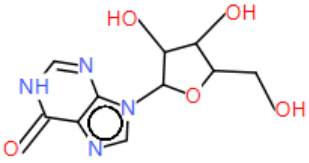
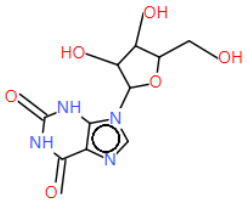
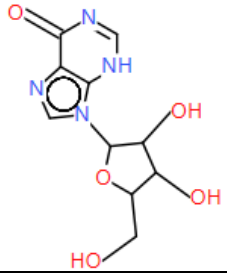
				(O)=O)ncnc21		
370			5-P-RIBOSYL-N-FORMYLGLYCINEAMIDE	OC1C(O)C(NC(=O)CNC=O)OC1COP(O)(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=5-P-RIBOSYL-N-FORMYLGLYCINEAMIDE
371	488-69-7		FRUCTOSE-16-DIPHOSPHATE	OC1C(O)C(O)(COP(O)(O)=O)OC1COP(O)(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=FRUCTOSE-16-DIPHOSPHATE
372	3672-15-9		MANNOSE-6P	OC1OC(COP(O)(O)=O)C(O)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=MANNOSE-6P
373	4300-28-1		RIBOSE-5P	OC1OC(COP(O)(O)=O)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=RIBOSE-5P
374	13270-65-0		PRPP	OC1C(O)C(OC1COP(O)(O)=O)OP(O)(=O)OP(O)(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=PRPP
375	576-37-4		GLUCURONATE	OC1OC(C(O)C(O)C1O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=GLUCURONATE

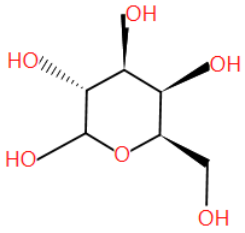
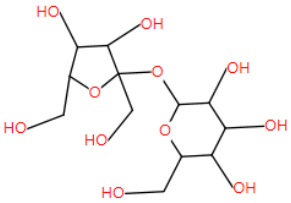
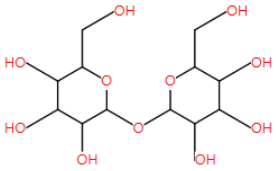
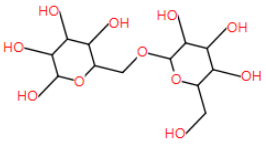
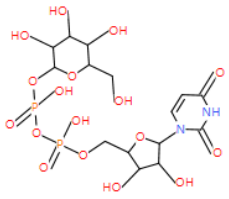
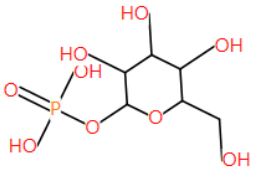
376	87-89-8		MYO-INOSITOL	OC1C(O)C(O)C(O)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=MYO-INOSITOL
377	46495-39-0		D-MYO-INOSITOL-4-PHOSPHATE	OC1C(O)C(O)C(OP(O)(O)=O)C(O)C1O		
378	126-49-8		PREPHENATE	OC1C=CC(CC(=O)C(O)=O)(C=C1)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=PREPHENATE
379			PYRROLINE-HYDROXY-CARBOXYLATE	OC1CC(N=C1)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=PYRROLINE-HYDROXY-CARBOXYLATE
380	51-35-4		L-4-HYDROXY-PROLINE	OC1CNC(C1)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=L-4-HYDROXY-PROLINE
381			Deoxyuridine triphosphate	OC1CC(OC1COP(O)(=O)OP(O)(=O)OP(O)(O)=O)N1C=CC(=O)NC1=O		
382			Deoxyuridine diphosphate	OC1CC(OC1COP(O)(=O)OP(O)(O)=O)N1C=CC(=O)NC1=O		
383			Deoxyuridine	c1cn(c(=O)nc1		

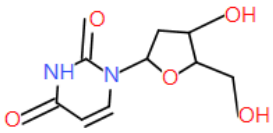
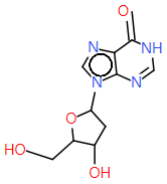
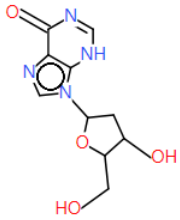
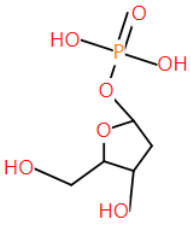
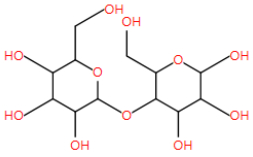
			monophosphate	O)[C@H]2C[C@@H]([C@H](O2)COP(=O)(O)O)O	 The structure is presented in the list of 427 predefined chemicals assumed as normal constituent of the body or an optical isomer of such.	
384	102916-66-5		DEOXY-RIBOSE-5P	OC1CC(O)C(COP(O)(O)=O)O1		http://biocyc.org/HUMAN/NEW-IMAGE?object=DEOXY-RIBOSE-5P
385	99-96-7	2028049	4-hydroxybenzoate	OC(=O)c1ccc(O)cc1		http://biocyc.org/HUMAN/NEW-IMAGE?object=4-hydroxybenzoate
386	156-39-8	2058529	P-HYDROXY-PHENYLPYRUVATE	OC(=O)C(=O)Cc1ccc(O)cc1		http://biocyc.org/HUMAN/NEW-IMAGE?object=P-HYDROXY-PHENYLPYRUVATE
387			34-DIHYDROXY PHENYLACETALDEHYDE	Oc1ccc(CC=O)cc1O		
388	1113-60-6		OH-PYR	OCC(=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=OH-PYR
389	2646-35-7		D-SEDOHEPTULOSE-7-P	OCC(=O)C(O)C(O)C(O)C(O)COP(O)(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=D-SEDOHEPTULOSE-7-P

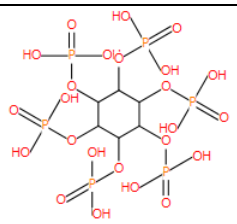
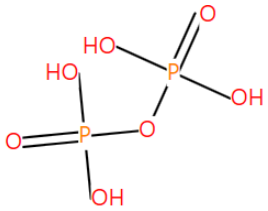
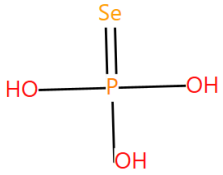
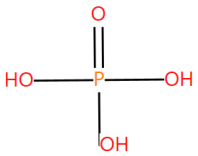
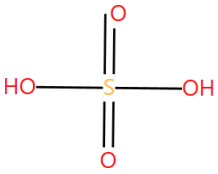
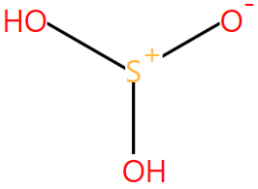
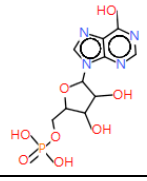
390	60802-29-1		XYLULOSE-5-PHOSPHATE	OCC(=O)C(O)C(O)COP(O)(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=XYLULOSE-5-PHOSPHATE
391	57-04-5	2003087	DIHYDROXY-ACETONE-PHOSPHATE	OCC(=O)COP(O)(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=DIHYDROXY-ACETONE-PHOSPHATE
392	2553-59-5		2-PG	OCC(OP(O)(O)=O)C(O)=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=2-PG
393	79-14-1	2011805	GLYCOLLATE	OCC(=O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=GLYCOLLATE
394	6000-40-4		GLYCERATE	[H]C(O)(CO)C(=O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=GLYCERATE
395	87-99-0		XYLITOL	OCC(O)C(O)C(O)CO		http://biocyc.org/HUMAN/NEW-IMAGE?object=XYLITOL
396	367-47-5		GLYCERALD	OCC(O)C=O		http://biocyc.org/HUMAN/NEW-IMAGE?object=GLYCERALD
397	50-81-7		ASCORBIC ACID	OC[C@H](O)[C@H]1OC(=O)C(O)=C1O		

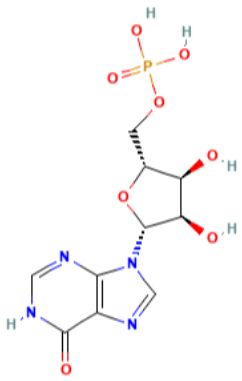
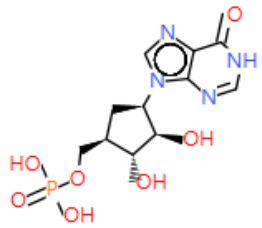
						
398	50-81-7	2000662	ASCORBATE	[H]C(O)(CO)C1([H])(OC(O)=C(O)C1(=O))		http://biocyc.org/HUMAN/NEW-IMAGE?object=ASCORBATE
399	56-81-5	2002895	GLYCEROL	OCC(O)CO		http://biocyc.org/HUMAN/NEW-IMAGE?object=GLYCEROL
400	57-03-4	2003071	GLYCEROL-3P	[H]C(O)(CO)COP(=O)(O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=GLYCEROL-3P
401	643-13-0		FRUCTOSE-6P	OCC1(O)OC(COP(O)(O)=O)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=FRUCTOSE-6P
402	551-84-8		D-XYLULOSE	[H]C1(O)(COC(O)(CO)C1([H])(O))		http://biocyc.org/HUMAN/NEW-IMAGE?object=D-XYLULOSE
403			CPD-535	[H]C1(O)(C([H])(O)C(CO)(OC1([H])(COP(=O)(O)O))OP(=O)(O)O)		http://biocyc.org/HUMAN/NEW-IMAGE?object=CPD-535
404	73023-76-4		HYDROXYMETHYLBILAN	OCC=4NC(CC=3NC(CC=2N		http://biocyc.org/HUMAN/NEW-

			E	C(CC=1NC=C(CCC(=O)O)C=1(CC(=O)O))=C(CCC(=O)O)C=2(CC(=O)O))=C(CCC(=O)O)C=3(CC(=O)O))=C(CCC(=O)O)C=4(CC(=O)O)		IMAGE?object=HYDROXYMETHYLBILANE
405	58-96-8	004075	URIDINE	OC[C@H]1O[C@@H](N2C=CC(=O)NC2=O)[C@H](O)[C@@H]1O		
406	58-63-9		INOSINE	[H]C3(CO)(OC([H])(N2C=NC=1C(=O)NC=NC=12)C([H])(O)C3([H])(O))		http://biocyc.org/HUMAN/NEW-IMAGE?object=INOSINE
407	146-80-5		XANTHOSINE	[H]C3(CO)(OC([H])(N2C=NC=1C(=O)NC(=O)NC=12)C([H])(O)C3([H])(O))		http://biocyc.org/HUMAN/NEW-IMAGE?object=XANTHOSINE
408	58-63-9		INOSINE_2	[H]C3(CO)(OC([H])(N2C=NC=1C(=O)N=CNC=12)C([H])(O)C3([H])(O))		

409	50-99-7		D-GLUCOSE	OC[C@H]1OC(O)[C@H](O)[C@@H](O)[C@@H]1O		
410	57-50-1		SUCROSE	[H]C2(O)(C([H])(O)C([H])(CO)OC([H])(OC1(CO)(OC([H])(CO)C([H])(O)C1([H])(O)))C2([H])(O))		http://biocyc.org/HUMAN/NEW-IMAGE?object=SUCROSE
411	99-20-7		TREHALOSE	[H]C2(O)(C([H])(O)C([H])(CO)OC([H])(OC1([H])(OC([H])(CO)C([H])(O)C([H])(O)C1([H])(O)))C2([H])(O))		http://biocyc.org/HUMAN/NEW-IMAGE?object=TREHALOSE
412	585-99-9		MELIBIOSE	[H]C2(O)(C(O)OC([H])(COC1([H])(OC([H])(CO)C([H])(O)C([H])(O)C1([H])(O)))C([H])(O)C2([H])(O))		http://biocyc.org/HUMAN/NEW-IMAGE?object=MELIBIOSE
413	2956-16-3		UDP-GALACTOSE	OCC1OC(OP(O)(=O)OP(O)(=O)OCC2OC(C(O)C2O)N2C=CC(=O)NC2=O)C(O)C(O)C1O		http://biocyc.org/HUMAN/NEW-IMAGE?object=UDP-GALACTOSE
414	2255-14-3		GALACTOSE-1P	[H]C1(O)(C([H])(O)C([H])(CO)OC([H])(OP(=O)(O)O)C1([H])(O))		http://biocyc.org/HUMAN/NEW-IMAGE?object=GALACTOSE-1P
415	951-78-0		DEOXYURIDINE	[H]C1(O)(CC([H])(OC1([H])(CO))N2C=CC		http://biocyc.org/HUMAN/NEW-IMAGE?object=D

				(=O)NC2(=O))		EOXYURIDINE
416	890-38-0		DEOXYINOSINE	[H]C1(O)(CC([H])(OC1([H])(CO))N3C=NC=2C(=O)NC=NC=23)		http://biocyc.org/HUMAN/NEW-IMAGE?object=DEOXYINOSINE
417	890-38-0		DEOXYINOSINE_2	[H]C1(O)(CC([H])(OC1([H])(CO))N3C=NC=2C(=O)N=CNC=23)		http://biocyc.org/HUMAN/NEW-IMAGE?object=DEOXYINOSINE
418	17210-42-3		DEOXY-RIBOSE-1P	[H]C1(O)(CC(OC1([H])(CO))OP(=O)(O)O)		http://biocyc.org/HUMAN/NEW-IMAGE?object=DEOXY-RIBOSE-1P
419	69-79-4		MALTOSE	[H]C2(O)(C(O)OC([H])(CO)C([H])(OC1([H])(OC([H])(CO)C([H])(O)C([H])(O)C1([H])(O)))C2([H])(O))		http://biocyc.org/HUMAN/NEW-IMAGE?object=MALTOSE
420	7722-84-1		HYDROGEN-PEROXIDE	OO		http://biocyc.org/HUMAN/NEW-IMAGE?object=HYDROGEN-PEROXIDE
421			MI-HEXAKISPHOSPHATE	O=P(O)(O)OC1C(OP(=O)(O)O)C(OP(=O)(O)O)C(OP(=O)(O)O)C(OP(=O)(O)O)C1(OP(=O)(O)O)		http://biocyc.org/HUMAN/NEW-IMAGE?object=MI-HEXAKISPHOSPHATE

						
422	2466-09-3	2195740	PPI	OP(=O)(O)OP(=O)(O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=PPI
423	16561-29-8		SEPO3	OP(O)(O)=[Se]		http://biocyc.org/HUMAN/NEW-IMAGE?object=SEPO3
424	14265-44-2		Pi	OP(=O)(O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=Pi
425	14808-79-8		SULFATE	OS(=O)(=O)O		http://biocyc.org/HUMAN/NEW-IMAGE?object=SULFATE
426	7782-99-2	2319731	SO3	O[S+](O)[O-]		http://biocyc.org/HUMAN/NEW-IMAGE?object=SO3
427	131-99-7		Inosine monophosphate	OC1C(COP(O)(O)=O)OC(C1O)n1cnc2c(O)ncnc12		https://www.tandfonline.com/doi/abs/10.1080/10629360802083871

428	131-99-7		Inosine monophosphate	C1=N[c]2[n](C3C(C(C(O3)COP(=O)([O])[O])[O])[O])[c][n][c]2C(=O)N1		https://pubchem.ncbi.nlm.nih.gov/compound/135398640
429	131-99-7		Inosine monophosphate	O[C@@H]1[C@@H](COP(O)(O)=O)C[C@H]([C@@H]1O)n1cnc2C(=O)NC=Nc12		https://www.tandfonline.com/doi/abs/10.1080/10629360802083871