AQ 肠菌 600 Pro 列表

ID	Compound Name	中文名称	缩写	CAS	Formula	Pubchem ID	HMDB ID	KEGG ID	Class	分类
1	Glycine	甘氨酸	Gly	56-40-6	C2H5NO2	750	HMDB0000123	C00037	Amino acid derivatives	氨基酸及其衍生物
2	L-Alanine	L-丙氨酸	Ala	56-41-7	C3H7NO2	5950	HMDB0000161	C00041	Amino acid derivatives	氨基酸及其衍生物
3	Gamma-Aminobutyric Acid	γ-氨基丁酸	GABA	56-12-2	C4H9NO2	119	HMDB0000112	C00334	Amino acid derivatives	氨基酸及其衍生物
4	Creatinine	肌酸酐	DADA	60-27-5	C4H7N3O	588	HMDB0000562	C00791	Amino acid derivatives	氨基酸及其衍生物
5	L-Proline	L-脯氨酸	Pro	147-85-3	C5H9NO2	145742	HMDB0000162	C00148	Amino acid derivatives	氨基酸及其衍生物
6	L-Valine	L-缬氨酸	Val	72-18-4	C5H11NO2	6287	HMDB0000883	C00183	Amino acid derivatives	氨基酸及其衍生物
7	L-Threonine	L-苏氨酸	Thr	72-19-5	C4H9NO3	6288	HMDB0000167	C00188	Amino acid derivatives	氨基酸及其衍生物
8	L-Cysteine	L-半胱氨酸	Cys	52-90-4	C3H7NO2S	5862	HMDB0000574	C00097	Amino acid derivatives	氨基酸及其衍生物
9	Creatine	肌酸	/	57-00-1	C4H9N3O2	586	HMDB0000064	C00300	Amino acid derivatives	氨基酸及其衍生物
10	trans-L-Hydroxyproline	trans-L-羟脯氨酸	Hyp	51-35-4	C5H9NO3	5810	HMDB0000725	C01157	Amino acid derivatives	氨基酸及其衍生物
11	L-Leucine	L-亮氨酸	Leu	61-90-5	C6H13NO2	6106	HMDB0000687	C00123	Amino acid derivatives	氨基酸及其衍生物
12	L-Isoleucine	L-异亮氨酸	Ile	73-32-5	C6H13NO2	6306	HMDB0000172	C00407	Amino acid derivatives	氨基酸及其衍生物
13	L-Ornithine	L-鸟氨酸	Orn	70-26-8	C5H12N2O2	6262	HMDB0000214	C00077	Amino acid derivatives	氨基酸及其衍生物
14	L-Asparagine	L-天冬酰胺	Asn	70-47-3	C4H8N2O3	6267	HMDB0000168	C00152	Amino acid derivatives	氨基酸及其衍生物
15	L-Aspartic acid	L-天冬氨酸	Asp	56-84-8	C4H7NO4	5960	HMDB0000191	C00049	Amino acid derivatives	氨基酸及其衍生物
16	L-Lysine	L-赖氨酸	Lys	56-87-1	C6H14N2O2	5962	HMDB0000182	C00047	Amino acid derivatives	氨基酸及其衍生物
17	L-Glutamine	L-谷氨酰胺	Gln	56-85-9	C5H10N2O3	5961	HMDB0000641	C00064	Amino acid derivatives	氨基酸及其衍生物
18	L-Methionine	L-甲硫氨酸	Met	63-68-3	C5H11NO2S	6137	HMDB0000696	C00073	Amino acid derivatives	氨基酸及其衍生物
19	L-Histidine	L-组氨酸	His	71-00-1	C6H9N3O2	6274	HMDB0000177	C00135	Amino acid derivatives	氨基酸及其衍生物

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20	L-Phenylalanine	L-苯丙氨酸	Phe	63-91-2	C9H11NO2	6140	HMDB0000159	C00079	Amino acid derivatives	氨基酸及其衍生物
21	1-Methyl-L-histidine	1-甲基-L-组氨酸	1-MHis	332-80-9	C7H11N3O2	92105	HMDB0000001	/	Amino acid derivatives	氨基酸及其衍生物
22	L-Arginine	L-精氨酸	Arg	74-79-3	C6H14N4O2	6322	HMDB0000517	C00062	Amino acid derivatives	氨基酸及其衍生物
23	L-Citrulline	L-瓜氨酸	Cit	372-75-8	C6H13N3O3	9750	HMDB0000904	C00327	Amino acid derivatives	氨基酸及其衍生物
24	L-Tyrosine	L-酪氨酸	Tyr	60-18-4	C9H11NO3	6057	HMDB0000158	C00082	Amino acid derivatives	氨基酸及其衍生物
25	O-Phospho-Serine	磷酸丝氨酸	/	407-41-0	C3H8NO6P	68841	HMDB0000272	C01005	Amino acid derivatives	氨基酸及其衍生物
26	Folic Acid	叶酸	/	59-30-3	C19H19N7O6	135398658	HMDB0000121	C00504	Amino acid derivatives	氨基酸及其衍生物
27	Sarcosine	肌氨酸	/	107-97-1	C3H7NO2	1088	HMDB0000271	C00213	Amino acid derivatives	氨基酸及其衍生物
28	Pyroglutamic acid	焦谷氨酸	PGA	98-79-3	C5H7NO3	7405	HMDB0000267	C01879	Amino acid derivatives	氨基酸及其衍生物
29	Aminohippuric acid	氨基马尿酸	/	61-78-9	C9H10N2O3	2148	HMDB0001867	D06890	Amino acid derivatives	氨基酸及其衍生物
30	N,N-Dimethylglycine	二甲基甘氨酸	DMG	1118-68-9	C4H9NO2	673	HMDB0000092	C01026	Amino acid derivatives	氨基酸及其衍生物
31	L-Serine	L-丝氨酸	Ser	56-45-1	C3H7NO3	5951	HMDB0000187	C00065	Amino acid derivatives	氨基酸及其衍生物
32	Aminolevulinic acid	5-氨基乙酰丙酸	/	106-60-5	C5H9NO3	137	HMDB0001149	C00430	Amino acid derivatives	氨基酸及其衍生物
33	6-Aminocaproic acid	6-氨基己酸	/	60-32-2	C6H13NO2	564	HMDB0001901	C02378	Amino acid derivatives	氨基酸及其衍生物
34	1-Methylnicotinamide	1-甲基烟酰胺	/	3106-60-3	C7H9N2O+	457	HMDB0000699	C02918	Amino acid derivatives	氨基酸及其衍生物
35	Cysteinesulfinic acid	半胱氨酸亚磺酸	/	1115-65-7	C3H7NO4S	1549098	HMDB0000996	C00606	Amino acid derivatives	氨基酸及其衍生物
36	5-Hydroxylysine	5-羟基赖氨酸	Hyl	1190-94-9	C6H14N2O3	3032849	HMDB0000450	C16741	Amino acid derivatives	氨基酸及其衍生物
37	L-Cysteic acid	L-半胱磺酸	/	498-40-8	C3H7NO5S	72886	HMDB0002757	C00506	Amino acid derivatives	氨基酸及其衍生物
38	Guanidinosuccinic acid	胍基琥珀酸	/	6133-30-8	C5H9N3O4	439918	HMDB0003157	C03139	Amino acid derivatives	氨基酸及其衍生物
39	Allantoic acid	尿囊酸	/	99-16-1	C4H8N4O4	203	HMDB0001209	C00499	Amino acid derivatives	氨基酸及其衍生物
40	Nicotinuric acid	烟酰甘氨酸	/	583-08-4	C8H8N2O3	68499	HMDB0003269	C05380	Amino acid derivatives	氨基酸及其衍生物
41	Salicyluric acid	2-羟基马尿酸	/	487-54-7	C9H9NO4	10253	HMDB0000840	C07588	Amino acid derivatives	氨基酸及其衍生物
42	Selenomethionine	硒甲硫氨酸	/	3211-76-5	C5H11NO2Se	105024	HMDB0003966	C05335	Amino acid derivatives	氨基酸及其衍生物
43	N-Acetyl-L-tyrosine	N-乙酰-L-酪氨酸	/	537-55-3	C11H13NO4	68310	HMDB0000866	C01657	Amino acid derivatives	氨基酸及其衍生物

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44	Phenylacetylglutamine	苯乙酰谷氨酰胺	/	28047-15-6	C13H16N2O4	92258	HMDB0006344	C04148	Amino acid derivatives	氨基酸及其衍生物
45	Saccharopine	酵母氨酸	/	997-68-2	C11H20N2O6	160556	HMDB0000279	C00449	Amino acid derivatives	氨基酸及其衍生物
46	2-Methylhippuric acid	2-甲基马尿酸	/	42013-20-7	C10H11NO3	91637	HMDB0011723	/	Amino acid derivatives	氨基酸及其衍生物
47	Phenylacetylglycine	苯乙酰甘氨酸	/	500-98-1	C10H11NO3	68144	HMDB0000821	C05598	Amino acid derivatives	氨基酸及其衍生物
48	Gamma-Glutamyl-Glutamate	γ-谷氨酰-谷氨酸	γ-Glu-Glu	1116-22-9	C10H16N2O7	92865	HMDB0011737	C05282	Amino acid derivatives	氨基酸及其衍生物
49	Glutathione	还原型谷胱甘肽	GSH	70-18-8	C10H17N3O6S	124886	HMDB0000125	C00051	Amino acid derivatives	氨基酸及其衍生物
50	Aspartyl-Lysine	天冬氨酰-赖氨酸	Asp-Lys	5891-51-0	C10H19N3O5	6427003	HMDB0004987	/	Amino acid derivatives	氨基酸及其衍生物
51	Xanthurenic acid	黄尿酸	Xa	59-00-7	C10H7NO4	5699	HMDB0000881	C02470	Amino acid derivatives	氨基酸及其衍生物
52	Cinnamoylglycine	肉桂酰甘氨酸	/	16534-24-0	C11H11NO3	709625	HMDB0011621	/	Amino acid derivatives	氨基酸及其衍生物
53	Threonyl-Phenylalanine	苏氨酰-苯丙氨酸	Thr-Phe	16875-27-7	C13H18N2O4	7010580	HMDB0029068	/	Amino acid derivatives	氨基酸及其衍生物
54	Guanidoacetic acid	胍乙酸	/	352-97-6	C3H7N3O2	763	HMDB0000128	C00581	Amino acid derivatives	氨基酸及其衍生物
55	beta-Alanine	β-丙氨酸	β-Ala	107-95-9	C3H7NO2	239	HMDB0000056	C00099	Amino acid derivatives	氨基酸及其衍生物
56	Maleamic Acid	马来酰胺酸	/	557-24-4	C4H5NO3	5280451	/	C01596	Amino acid derivatives	氨基酸及其衍生物
57	2-Aminoisobutyric acid	2-氨基异丁酸	/	62-57-7	C4H9NO2	6119	HMDB0001906	C03665	Amino acid derivatives	氨基酸及其衍生物
58	L-Homocysteine	L-高半胱氨酸	/	6027-13-0	C4H9NO2S	91552	HMDB0000742	C00155	Amino acid derivatives	氨基酸及其衍生物
59	5-Aminovaleric acid	5-氨基戊酸	/	660-88-8	C5H11NO2	138	HMDB0003355	C00431	Amino acid derivatives	氨基酸及其衍生物
60	N-Acetyl-L-alanine	N-乙酰-L-丙氨酸	/	97-69-8	C5H9NO3	88064	HMDB0000766	/	Amino acid derivatives	氨基酸及其衍生物
61	N-Acetyl-L-cysteine	N-乙酰-L-半胱氨酸	/	616-91-1	C5H9NO3S	12035	HMDB0001890	C06809	Amino acid derivatives	氨基酸及其衍生物
62	L-Glutamic acid	L-谷氨酸	Glu	56-86-0	C5H9NO4	33032	HMDB0000148	C00025	Amino acid derivatives	氨基酸及其衍生物
63	N-Methyl-L-glutamic acid	N-甲基-L-谷氨酸	/	35989-16-3	C6H11NO4	439377	HMDB0062660	C01046	Amino acid derivatives	氨基酸及其衍生物
64	L-Cystine	L-胱氨酸	Cys	56-89-3	C6H12N2O4S2	67678	HMDB0000192	C00491	Amino acid derivatives	氨基酸及其衍生物
65	L-Kynurenine	L-犬尿氨酸	Kyn	2922-83-0	C10H12N2O3	161166	HMDB0000684	C00328	Amino acid derivatives	氨基酸及其衍生物
66	N-Acetyl-L-aspartic acid	N-乙酰-L-天冬氨酸	/	997-55-7	C6H9NO5	65065	HMDB0000812	C01042	Amino acid derivatives	氨基酸及其衍生物
67	N-Acetyl-L-glutamine	N-乙酰-L-谷氨酰胺	/	2490-97-3	C7H12N2O4	182230	HMDB0006029	D07063	Amino acid derivatives	氨基酸及其衍生物

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68	L-Homocitrulline	L-高瓜氨酸	/	1190-49-4	C7H15N3O3	65072	HMDB0000679	C02427	Amino acid derivatives	氨基酸及其衍生物
69	L-Homoarginine	L-高精氨酸	/	156-86-5	C7H16N4O2	9085	HMDB0000670	C01924	Amino acid derivatives	氨基酸及其衍生物
70	2-Aminooctanoic acid	2-氨基辛酸	/	644-90-6	C8H17NO2	69522	HMDB0000991	/	Amino acid derivatives	氨基酸及其衍生物
71	Levodopa	左旋多巴	L-DOPA	59-92-7	C9H11NO4	6047	HMDB0000181	C00355	Amino acid derivatives	氨基酸及其衍生物
72	L-Carnosine	L-肌肽	/	305-84-0	C9H14N4O3	439224	HMDB0000033	C00386	Amino acid derivatives	氨基酸及其衍生物
73	Hippuric acid	马尿酸	HA	495-69-2	C9H9NO3	464	HMDB0000714	C01586	Amino acid derivatives	氨基酸及其衍生物
74	3-Hydroxykynurenine	3-羟基犬尿氨酸	3-HK	2147-61-7	C10H12N2O4	89	HMDB0000732	C02794	Amino acid derivatives	氨基酸及其衍生物
75	L-2-Aminoadipic acid	L-2-氨基己二酸	/	1118-90-7	C6H11NO4	92136	HMDB0000510	C00956	Amino acid derivatives	氨基酸及其衍生物
76	3-Aminoisobutyric acid	3-氨基异丁酸	/	144-90-1	C4H9NO2	64956	HMDB0003911	C05145	Amino acid derivatives	氨基酸及其衍生物
77	Norvaline	正缬氨酸	/	6600-40-4	C5H11NO2	65098	HMDB0251527	C01826	Amino acid derivatives	氨基酸及其衍生物
78	S-Methyl-cysteine	S-甲基-半胱氨酸	/	1187-84-4	C4H9NO2S	24417	HMDB0302211	C22040	Amino acid derivatives	氨基酸及其衍生物
79	2-Phenylglycine	2-苯甘氨酸	/	2835-06-5	C8H9NO2	3866	HMDB0002210	/	Amino acid derivatives	氨基酸及其衍生物
80	N-Acetyl-L-leucine	N-乙酰-L-亮氨酸	/	99-15-0	C8H15NO3	1995	HMDB0341345	C02710	Amino acid derivatives	氨基酸及其衍生物
81	N-(2-Furoyl)glycine	N -(2 -呋喃甲酰基)甘氨酸	/	5657-19-2	C7H7NO4	21863	HMDB0000439	/	Amino acid derivatives	氨基酸及其衍生物
82	Gamma-Glutamyl-Valine	γ-谷氨酰-缬氨酸	γ-Glu-Val	2746-34-1	C10H18N2O5	7015683	HMDB0011172	/	Amino acid derivatives	氨基酸及其衍生物
83	5-Hydroxytryptophan	5-羟色氨酸	5-HTP	56-69-9	C11H12N2O3	144	HMDB0000472	C00643	Amino acid derivatives	氨基酸及其衍生物
84	3-Nitrotyrosine	3-硝基酪氨酸	/	621-44-3	C9H10N2O5	65124	HMDB0001904	C22981	Amino acid derivatives	氨基酸及其衍生物
85	Tiglylglycine	巴豆酰甘氨酸	/	35842-45-6	C7H11NO3	6441567	HMDB0000959	/	Amino acid derivatives	氨基酸及其衍生物
86	4-Hydroxyhippuric acid	4-羟基马尿酸	/	2482-25-9	C9H9NO4	151012	HMDB0013678	/	Amino acid derivatives	氨基酸及其衍生物
87	3-Methoxytyrosine	3-甲氧基酪氨酸	/	7636-26-2	C10H13NO4	1670	HMDB0001434	/	Amino acid derivatives	氨基酸及其衍生物
88	3-Hydroxyhippuric acid	3-羟基马尿酸	/	1637-75-8	C9H9NO4	450268	HMDB0006116	/	Amino acid derivatives	氨基酸及其衍生物
89	4-Acetamidobutyric acid	4-乙酰氨基丁酸	/	3025-96-5	C6H11NO3	18189	HMDB0003681	C02946	Amino acid derivatives	氨基酸及其衍生物
90	L-Proline betaine	L-水苏碱	/	471-87-4	C7H13NO2	115244	HMDB0004827	C10172	Amino acid derivatives	氨基酸及其衍生物
91	Aspartyl-phenylalanine	天冬氨酰-苯丙氨酸	/	13433-09-5	C13H16N2O5	93078	HMDB0000706	/	Amino acid derivatives	氨基酸及其衍生物

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92	4-Hydroxyphenylacetylglycine	4-羟基苯乙酰基甘氨酸	/	28116-23-6	C10H11NO4	440732	HMDB0000735	C05596	Amino acid derivatives	氨基酸及其衍生物
93	5-Glutamyl-Taurine	5-谷氨酰-牛磺酸	/	56488-60-9	C7H14N2O6S	68759	HMDB0004195	C05844	Amino acid derivatives	氨基酸及其衍生物
94	Glycyl-Glycine	甘氨酰-甘氨酸	Gly-Gly	556-50-3	C4H8N2O3	11163	HMDB0011733	C02037	Amino acid derivatives	氨基酸及其衍生物
95	3-Chlorotyrosine	3-氯酪氨酸	/	7423-93-0	C9H10ClNO3	110992	/	/	Amino acid derivatives	氨基酸及其衍生物
96	N-Methylproline	N-甲基脯氨酸	/	68078-09-1	C6H11NO2	557	HMDB0242151	/	Amino acid derivatives	氨基酸及其衍生物
97	Tryptophanamide	色氨酸酰胺	/	20696-57-5	C11H13N3O	439356	/	C00977	Amino acid derivatives	氨基酸及其衍生物
98	N-Acetyl-L-tryptophan	N-乙酰-L-色氨酸	/	1218-34-4	C13H14N2O3	700653	HMDB0013713	/	Amino acid derivatives	氨基酸及其衍生物
99	Glycyl-Valine	甘氨酰-缬氨酸	Gly-Val	2325-17-9	C7H14N2O3	97417	/	/	Amino acid derivatives	氨基酸及其衍生物
100	Thyronine	甲状腺原氨酸	/	1596-67-4	C15H15NO4	5461103	HMDB0000667	/	Amino acid derivatives	氨基酸及其衍生物
101	Ophthalmic Acid	眼氨酸	/	495-27-2	C11H19N3O6	7018721	HMDB0005765	C21016	Amino acid derivatives	氨基酸及其衍生物
102	Phenylpropionylglycine	苯丙酰-甘氨酸	/	56613-60-6	C11H13NO3	152323	HMDB0000860	/	Amino acid derivatives	氨基酸及其衍生物
103	Gamma-Glutamyl-Tyrosine	γ-谷氨酰-酪氨酸	γ-Glu-Tyr	7432-23-7	C14H18N2O6	94340	HMDB0011741	/	Amino acid derivatives	氨基酸及其衍生物
104	Isovalerylglutamic Acid	异戊酰谷氨酸	/	80154-63-8	C10H17NO5	133383	HMDB0000726	/	Amino acid derivatives	氨基酸及其衍生物
105	Alpha-Hydroxyhippuric Acid	α-羟基马尿酸	/	16555-77-4	C9H9NO4	450272	HMDB0002404	/	Amino acid derivatives	氨基酸及其衍生物
106	Leucyl-Glycine	亮氨酰-甘氨酸	Leu-Gly	686-50-0	C8H16N2O3	97364	/	/	Amino acid derivatives	氨基酸及其衍生物
107	Alanyl-Glycine	丙氨酰-甘氨酸	Ala-Gly	687-69-4	C5H10N2O3	6998028	HMDB0006899	/	Amino acid derivatives	氨基酸及其衍生物
108	N-Octanoylglycine	辛酰甘氨酸	/	14246-53-8	C10H19NO3	84290	HMDB0000832	/	Amino acid derivatives	氨基酸及其衍生物
109	Glutamyl-Cysteine	谷氨酰-半胱氨酸	Glu-Cys	21566-73-4	C8H14N2O5S	10171468	HMDB0028816	/	Amino acid derivatives	氨基酸及其衍生物
110	Gamma-Glutamyl-Isoleucine	γ-谷氨酰-异亮氨酸	γ-Glu-Ile	5879-22-1	C11H20N2O5	9813855	HMDB0028822	/	Amino acid derivatives	氨基酸及其衍生物
111	Aspartyl-Glutamic Acid	天冬氨酰-谷氨酸	Asp-Glu	6157-06-8	C9H14N2O7	151403	/	/	Amino acid derivatives	氨基酸及其衍生物
112	Gamma-Glutamyl-Glutamine	γ-谷氨酰-谷氨酰胺	γ-Glu-Gln	10148-81-9	C10H17N3O6	150914	HMDB0011738	C05283	Amino acid derivatives	氨基酸及其衍生物
113	Isoleucyl-Serine	异亮氨酰-丝氨酸	Ile-Ser	6403-14-1	C9H18N2O4	7021816	/	/	Amino acid derivatives	氨基酸及其衍生物
114	Aspartyl-Leucine	天冬氨酰-亮氨酸	Asp-Leu	3062-14-4	C10H18N2O5	6992367	/	/	Amino acid derivatives	氨基酸及其衍生物
115	Glutamyl-Lysine	谷氨酰-赖氨酸	Glu-Lys	5891-53-2	C11H21N3O5	7015704	HMDB0004207	/	Amino acid derivatives	氨基酸及其衍生物

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116	Phenylalanyl-Glutamate	苯丙氨酰-谷氨酸	Phe-Glu	3617-45-6	C14H18N2O5	151134	HMDB0028994	/	Amino acid derivatives	氨基酸及其衍生物
117	Leucyl-Proline	亮氨酰-脯氨酸	Leu-Pro	6403-35-6	C11H20N2O3	80817	HMDB0011175	/	Amino acid derivatives	氨基酸及其衍生物
118	Aspartyl-Alanine	天冬氨酰-丙氨酸	Asp-Ala	13433-02-8	C7H12N2O5	5491963	/	/	Amino acid derivatives	氨基酸及其衍生物
119	N-Decanoylglycine	N-癸酰甘氨酸	/	14305-32-9	C12H23NO3	1712391	HMDB0013267	/	Amino acid derivatives	氨基酸及其衍生物
120	N-Nonanoylglycine	N-壬酰甘氨酸	/	79251-60-8	C11H21NO3	10176752	HMDB0013279	/	Amino acid derivatives	氨基酸及其衍生物
121	Deoxycholic acid	脱氧胆酸	DCA	83-44-3	C24H40O4	222528	HMDB0000626	C04483	Bile acids	胆汁酸类
122	Cholic acid	胆酸	CA	81-25-4	C24H40O5	221493	HMDB0000619	C00695	Bile acids	胆汁酸类
123	Taurodeoxycholic acid	牛磺脱氧胆酸	TDCA	516-50-7	C26H45NO6S	2733768	HMDB0000896	C05463	Bile acids	胆汁酸类
124	Glycocholic acid	甘氨胆酸	GCA	475-31-0	C26H43NO6	10140	HMDB0000138	C01921	Bile acids	胆汁酸类
125	Glycolithocholic acid	甘氨石胆酸	GLCA	474-74-8	C26H43NO4	115245	HMDB0000698	C15557	Bile acids	胆汁酸类
126	Glycodeoxycholic acid	甘氨脱氧胆酸	GDCA	360-65-6	C26H43NO5	22833539	HMDB0000631	C05464	Bile acids	胆汁酸类
127	Taurolithocholic acid	牛磺石胆酸	TLCA	6042-32-6	C26H45NO5S	53477716	HMDB0000722	C02592	Bile acids	胆汁酸类
128	Taurochenodeoxycholic acid	牛磺鹅脱氧胆酸	TCDCA	516-35-8	C26H45NO6S	387316	HMDB0000951	C05465	Bile acids	胆汁酸类
129	23-Nordeoxycholic acid	23-脱甲脱氧胆酸	23-norDCA	53608-86-9	C23H38O4	193905	/	/	Bile acids	胆汁酸类
130	Dehydrocholic acid	脱氢胆酸	DHCA	81-23-2	C24H34O5	6674	/	C13154	Bile acids	胆汁酸类
131	7,12-Diketolithocholic acid	7,12-二酮石胆酸	7,12-diketoLCA	517-33-9	C24H36O5	3080560	/	/	Bile acids	胆汁酸类
132	6,7-Diketolithocholic acid	6,7-二酮石胆酸	6,7-diketoLCA	1643669-23-1	C24H36O5	137333800	/	/	Bile acids	胆汁酸类
133	Dehydrolithocholic acid	脱氢石胆酸	DHLCA	1553-56-6	C24H38O3	5283906	/	C03070	Bile acids	胆汁酸类
134	12-Ketolithocholic acid	12-酮石胆酸	12-KLCA	5130-29-0	C24H38O4	3080612	HMDB0000328	/	Bile acids	胆汁酸类
135	7-Ketolithocholic acid	7-酮石胆酸	7-KLCA	4651-67-6	C24H38O4	444262	HMDB0000467	/	Bile acids	胆汁酸类
136	Apocholic acid	原胆酸	apoCA	641-81-6	C24H38O4	101818	/	C15375	Bile acids	胆汁酸类
137	12-Dehydrocholic acid	12-脱氢胆酸	12-DHCA	2458-08-4	C24H38O5	94235	HMDB0000400	/	Bile acids	胆汁酸类
138	3-Dehydrocholic acid	3-脱氢胆酸	3-DHCA	2304-89-4	C24H38O5	5283956	HMDB0000502	/	Bile acids	胆汁酸类
139	7-Ketodeoxycholic acid	7-酮脱氧胆酸	7-KDCA	911-40-0	C24H38O5	188292	HMDB0000391	C04643	Bile acids	胆汁酸类

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140	Isolithocholic acid	异石胆酸	isoLCA	1534-35-6	C24H40O3	164853	HMDB0000717	C17658	Bile acids	胆汁酸类
141	Lithocholic acid	石胆酸	LCA	434-13-9	C24H40O3	9903	HMDB0000761	C03990	Bile acids	胆汁酸类
142	Ursodeoxycholic acid	熊脱氧胆酸	UDCA	128-13-2	C24H40O4	31401	HMDB0000946	C07880	Bile acids	胆汁酸类
143	Hyodeoxycholic acid	猪脱氧胆酸	HDCA	83-49-8	C24H40O4	5283820	HMDB0000733	C15517	Bile acids	胆汁酸类
144	Isodeoxycholic acid	异脱氧胆酸	isoDCA	566-17-6	C24H40O4	164672	HMDB0002536	C17661	Bile acids	胆汁酸类
145	Chenodeoxycholic acid	鹅脱氧胆酸	CDCA	474-25-9	C24H40O4	10133	HMDB0000518	C02528	Bile acids	胆汁酸类
146	Ursocholic acid	熊果胆酸	UCA	2955-27-3	C24H40O5	122340	HMDB0000917	C17644	Bile acids	胆汁酸类
147	alpha-Muricholic acid	α-鼠胆酸	α-MCA	2393-58-0	C24H40O5	5283852	HMDB0000506	C17647	Bile acids	胆汁酸类
148	Hyocholic acid	猪胆酸	HCA	547-75-1	C24H40O5	92805	HMDB0000760	C17649	Bile acids	胆汁酸类
149	beta-Muricholic acid	β-鼠胆酸	β-MCA	2393-59-1	C24H40O5	5283853	HMDB0000415	C17726	Bile acids	胆汁酸类
150	Glycodehydrocholic acid	甘氨脱氢胆酸	GDHCA	3415-45-0	C26H37NO6	13955640	/	/	Bile acids	胆汁酸类
151	Glycochenodeoxycholic acid	甘氨鹅脱氧胆酸	GCDCA	640-79-9	C26H43NO5	12544	HMDB0000637	C05466	Bile acids	胆汁酸类
152	Glycoursodeoxycholic acid	甘氨熊脱氧胆酸	GUDCA	64480-66-6	C26H43NO5	12310288	HMDB0000708	/	Bile acids	胆汁酸类
153	Glycohyodeoxycholic acid	甘氨猪脱氧胆酸	GHDCA	13042-33-6	C26H43NO5	114611	HMDB0304944	/	Bile acids	胆汁酸类
154	Glycohyocholic acid	甘氨猪胆酸	GHCA	32747-08-3	C26H43NO6	71361462	HMDB0240607	/	Bile acids	胆汁酸类
155	Tauroursodeoxycholic acid	牛磺熊脱氧胆酸	TUDCA	14605-22-2	C26H45NO6S	9848818	HMDB0000874	C16868	Bile acids	胆汁酸类
156	Taurohyodeoxycholic acid	牛磺猪脱氧胆酸	THDCA	2958-04-5	C26H45NO6S	119046	/	/	Bile acids	胆汁酸类
157	Taurocholic acid	牛磺胆酸	TCA	81-24-3	C26H45NO7S	6675	HMDB0000036	C05122	Bile acids	胆汁酸类
158	Tauro beta-Muricholic acid	牛磺-β-鼠胆酸	T-β-MCA	25696-60-0	C26H45NO7S	21124703	HMDB0000932	/	Bile acids	胆汁酸类
159	Tauro alpha-Muricholic acid	牛磺-α-鼠胆酸	T-α-MCA	25613-05-2	C26H45NO7S	101657566	/	/	Bile acids	胆汁酸类
160	Taurohyocholic acid	牛磺猪胆酸	THCA	32747-07-2	C26H45NO7S	11954195	HMDB0011637	C15516	Bile acids	胆汁酸类
161	Murideoxycholic acid	鼠脱氧胆酸	MDCA	668-49-5	C24H40O4	5283821	HMDB00811	C15515	Bile acids	胆汁酸类
162	Isoursodeoxycholic acid	异熊脱氧胆酸	isoUDCA	78919-26-3	C24H40O4	127601	HMDB00686	C17662	Bile acids	胆汁酸类
163	Isohyodeoxycholic acid	异猪脱氧胆酸	isoHDCA	570-84-3	C24H40O4	5283822	HMDB00664	/	Bile acids	胆汁酸类

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164	3-Epideoxycholic acid	3β-脱氧胆酸	3β-DCA	570-63-8	C24H40O4	160530	HMDB00438	C20865	Bile acids	胆汁酸类
165	Lithocholic Acid-3-Sulfate	石胆酸硫酸	LCA-3S	64936-81-8	C24H40O6S	451489	HMDB00907	/	Bile acids	胆汁酸类
166	Ursodeoxycholic Acid-3-Sulfate	熊脱氧胆酸-3-硫酸	UDCA-3S	68780-73-4	C24H40O7S	9826093	HMDB0002642	/	Bile acids	胆汁酸类
167	Glycochenodeoxycholic acid 3-Sulfate	甘氨鹅脱氧胆酸-3-硫酸	GCDCA-3S	66874-09-7	C26H43NO8S	171818	HMDB0002497	/	Bile acids	胆汁酸类
168	Chenodeoxycholic acid 24-Acyl-β -D-glucuronide	鹅脱氧胆酸-24-酰基-β-葡糖苷酸	CDCA-24G	208038-27-1	C30H48O10	71314663	/	/	Bile acids	胆汁酸类
169	Chenodeoxycholic acid-3-β -D-Glucuronide	鹅脱氧胆酸-3-β-葡糖苷酸	CDCA-3G	58814-71-4	C30H48O10	21252299	HMDB0002430	/	Bile acids	胆汁酸类
170	Glycodeoxycholic acid-3-O-β-glucuronide	甘氨脱氧胆酸-3-O-β-葡糖苷酸	GDCA-3G	75672-36-5	C32H51NO11	169441040	/	/	Bile acids	胆汁酸类
171	Glycochenodeoxycholic Acid-3-O-β -glucuronide	甘氨鹅脱氧胆酸-3-O-β-葡糖醛酸	GCDCA-3G	75672-22-9	C32H51NO11	44263370	/	/	Bile acids	胆汁酸类
172	3beta-Cholic acid	3β-胆酸	3β-CA	3338-16-7	C24H40O5	5283870	HMDB0000419	/	Bile acids	胆汁酸类
173	6-Ketolithocholic acid	6-酮石胆酸	6-KLCA	2393-61-5	C24H38O4	164960	/	/	Bile acids	胆汁酸类
174	Norcholic acid	去甲胆酸	NCA	60696-62-0	C23H38O5	158738	HMDB0255727	/	Bile acids	胆汁酸类
175	Taurolithocholic Acid-3-Sulfate	牛磺石胆酸-3-硫酸	TLCA-3S	15324-65-9	C26H45NO8S2	440071	HMDB0002580	C03642	Bile acids	胆汁酸类
176	Glycolithocholic Acid-3-Sulfate	甘氨石胆酸-3-硫酸	GLCA-3S	15324-64-8	C26H43NO7S	72222	HMDB0002639	/	Bile acids	胆汁酸类
177	Glycodeoxycholic Acid-3-Sulfate	甘氨脱氧胆酸-3-硫酸	GDCA-3S	66874-10-0	C26H43NO8S	101602538	HMDB0341325	/	Bile acids	胆汁酸类
178	Cholic Acid-3-Sulfate	胆酸-3-硫酸	CA-3S	58822-34-7	C24H40O8S	465402	/	/	Bile acids	胆汁酸类
179	Glycocholic Acid-3-Sulfate	甘氨胆酸-3-硫酸	GCA-3S	67850-84-4	C26H43NO9S	101602537	HMDB0240728	/	Bile acids	胆汁酸类
180	Taurocholic Acid-3-Sulfate	牛磺胆酸-3-硫酸	TCA-3S	67030-62-0	C26H45NO10S2	14454428	HMDB0002581	/	Bile acids	胆汁酸类
181	Deoxycholic Acid-3-Sulfate	脱氧胆酸-3-硫酸	DCA-3S	67030-48-2	C24H40O7S	128752	HMDB0002504	/	Bile acids	胆汁酸类
182	Taurodeoxycholic Acid-3-Sulfate	牛磺脱氧胆酸-3-硫酸	TDCA-3S	/	C26H45NO9S2	21252302	HMDB0341535	/	Bile acids	胆汁酸类
183	Chenodeoxycholic Acid-3-Sulfate	鹅脱氧胆酸-3-硫酸	CDCA-3S	59132-32-0	C24H40O7S	21252312	HMDB0002586	/	Bile acids	胆汁酸类
184	Taurochenodeoxycholic Acid-3-Sulfate	牛磺鹅脱氧胆酸-3-硫酸	TCDCA-3S	67030-59-5	C26H45NO9S2	194244	HMDB0002486	/	Bile acids	胆汁酸类

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185	Glycoursodeoxycholic Acid-3-Sulfate	甘氨熊脱氧胆酸-3-硫酸	GUDCA-3S	133429-88-6	C26H43NO8S	21116917	HMDB0002409	/	Bile acids	胆汁酸类
186	Tauroursodeoxycholic Acid-3-Sulfate	牛磺熊脱氧胆酸-3-硫酸	TUDCA-3S	/	C26H45NO9S2	101931089	HMDB0002504	/	Bile acids	胆汁酸类
187	3-Oxo-4,6-Choladienoate	3-氧代-4,6-胆二烯酸	/	88179-71-9	C24H34O3	5283992	HMDB0000476	/	Bile acids	胆汁酸类
188	Acetic acid	乙酸	/	64-19-7	CH3COOH	176	HMDB0000042	C00033	Short-chain fatty acid	短链脂肪酸
189	Propanoic acid	丙酸	/	79-09-4	C3H6O2	1032	HMDB0000237	C00163	Short-chain fatty acid	短链脂肪酸
190	Butyric acid	丁酸	/	107-92-6	C4H8O2	264	HMDB0000039	C00246	Short-chain fatty acid	短链脂肪酸
191	Isobutyric acid	异丁酸	/	79-31-2	C4H8O2	6590	HMDB0001873	C02632	Short-chain fatty acid	短链脂肪酸
192	Valeric acid	戊酸	/	109-52-4	C5H10O2	7991	HMDB0000892	C00803	Short-chain fatty acid	短链脂肪酸
193	Isovaleric acid	异戊酸	/	503-74-2	C5H10O2	10430	HMDB0000718	C08262	Short-chain fatty acid	短链脂肪酸
194	Hexanoic acid	己酸	/	142-62-1	C6H12O2	8892	HMDB0000535	C01585	Short-chain fatty acid	短链脂肪酸
195	Heptanoic acid	庚酸	/	111-14-8	C7H14O2	8094	HMDB0000666	C17714	Fatty Acids	脂肪酸类
196	Octanoic acid	辛酸	FA(8:0)	124-07-2	C8H16O2	379	HMDB0000482	C06423	Fatty Acids	脂肪酸类
197	Nonanoic acid	壬酸	FA(9:0)	112-05-0	C9H18O2	8158	HMDB0000847	C01601	Fatty Acids	脂肪酸类
198	Decanoic Acid	癸酸	FA(10:0)	334-48-5	C10H20O2	2969	HMDB0000511	C01571	Fatty Acids	脂肪酸类
199	Methylglutaric acid	甲基戊二酸	/	626-51-7	C6H10O4	12284	HMDB0000752	/	Fatty Acids	脂肪酸类
200	Lauric acid	十二烷酸（月桂酸）	FA(12:0)	143-07-7	C12H24O2	3893	HMDB0000638	C02679	Fatty Acids	脂肪酸类
201	Myristic Acid	十四烷酸（肉豆蔻酸）	FA(14:0)	544-63-8	C14H28O2	11005	HMDB0000806	C06424	Fatty Acids	脂肪酸类
202	Pentadecanoic Acid	十五烷酸	FA(15:0)	1002-84-2	C15H30O2	13849	HMDB0000826	C16537	Fatty Acids	脂肪酸类
203	Palmitic Acid	十六烷酸（棕榈酸）	FA(16:0)	57-10-3	C16H32O2	985	HMDB0000220	C00249	Fatty Acids	脂肪酸类
204	Undecanedioate	十一烷二酸	/	1852-04-6	C11H20O4	15816	HMDB0000888	/	Fatty Acids	脂肪酸类
205	Dodecanedioic acid	十二烷二酸	FA(12:1;O2)	693-23-2	C12H22O4	12736	HMDB0000623	C02678	Fatty Acids	脂肪酸类
206	Octadecanedioic acid	十八烷二酸	/	871-70-5	C18H34O4	70095	HMDB0000782	/	Fatty Acids	脂肪酸类
207	3-Hexenedioic Acid	3-己烯二酸	/	4436-74-2	C6H8O4	5351896	HMDB0000393	/	Fatty Acids	脂肪酸类
208	3-Methylglutaconic Acid	3-甲基戊烯二酸	/	5746-90-7	C6H8O4	1551553	HMDB0000522	/	Fatty Acids	脂肪酸类

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209	Palmitoleic acid	顺式-9-棕榈油酸	FA(16:1)	373-49-9	C16H30O2	445638	HMDB0003229	C08362	Fatty Acids	脂肪酸类
210	alpha-Linolenic acid	α-亚麻酸	FA(18:3)/ALA	463-40-1	C18H30O2	5280934	HMDB0001388	C06427	Fatty Acids	脂肪酸类
211	Oleic acid	顺式-9-十八碳烯酸（油酸）	FA(18:1)	112-80-1	C18H34O2	445639	HMDB0000207	C00712	Fatty Acids	脂肪酸类
212	Eicosapentaenoic acid	二十碳五烯酸	EPA	10417-94-4	C20H30O2	5282847	HMDB0001999	C06428	Fatty Acids	脂肪酸类
213	Arachidonic acid	花生四烯酸	ARA	506-32-1	C20H32O2	444899	HMDB0001043	C00219	Fatty Acids	脂肪酸类
214	Linoleic acid	顺式-9,12-亚油酸	FA(18:2)/LA	60-33-3	C18H32O2	5280450	HMDB0000673	C01595	Fatty Acids	脂肪酸类
215	Docosahexaenoic acid	二十二碳六烯酸	DHA	6217-54-5	C22H32O2	445580	HMDB0002183	C06429	Fatty Acids	脂肪酸类
216	Adrenic acid	二十二碳四烯酸	DTA	28874-58-0	C22H36O2	5497181	HMDB0002226	C16527	Fatty Acids	脂肪酸类
217	cis-8,11,14-eicosatrienoic acid	顺式-8,11,14-二十碳三烯酸	FA(20:3)/DGLA	1783-84-2	C20H34O2	5280581	HMDB0002925	C03242	Fatty Acids	脂肪酸类
218	Docosapentaenoic acid	二十二碳五烯酸	FA(22:5)/DPA	24880-45-3	C22H34O2	5497182	HMDB0006528	C16513	Fatty Acids	脂肪酸类
219	Carnitine	肉碱	CAR-OH	541-15-1	C7H15NO3	10917	HMDB0000062	C00318	Carnitines	肉碱类
220	Palmitoylcarnitine	棕榈酰肉碱	/	2364-67-2	C23H45NO4	11953816	HMDB0240774	C02990	Carnitines	肉碱类
221	Acetylcarnitine	乙酰肉碱	/	3040-38-8	C9H17NO4	7045767	HMDB0000201	C02571	Carnitines	肉碱类
222	Propionylcarnitine	丙酰肉碱	/	20064-19-1	C10H19NO4	107738	HMDB0000824	C03017	Carnitines	肉碱类
223	Butyrylcarnitine	丁酰肉碱	/	25576-40-3	C11H21NO4	213144	HMDB0002013	C02862	Carnitines	肉碱类
224	Lauroylcarnitine	月桂酰肉碱	/	25518-54-1	C19H37NO4	168381	HMDB0002250	/	Carnitines	肉碱类
225	Isovalerylcaritine	异戊酰肉碱	/	139144-12-0	C12H23NO4	6426851	HMDB0000688	C20826	Carnitines	肉碱类
226	Tiglylcarnitine	顺芷酰肉碱	/	64681-36-3	C12H21NO4	22833596	HMDB0002366	/	Carnitines	肉碱类
227	Malonylcarnitine	丙二酰肉碱	/	853728-01-5	C10H17NO6	71464475	HMDB0002095	/	Carnitines	肉碱类
228	Ethanolamine	乙醇胺	/	141-43-5	C2H7NO	700	HMDB0000149	C00189	Biogenic Amines	生物胺类
229	Choline	胆碱	Choline	62-49-7	C5H14NO	305	HMDB0000097	C00114	Biogenic Amines	生物胺类
230	Betaine	甜菜碱	Bet	107-43-7	C5H11NO2	247	HMDB0000043	C00719	Biogenic Amines	生物胺类
231	Acetylputrescine	乙酰腐胺	/	5699-41-2	C6H14N2O	122356	HMDB0002064	C02714	Biogenic Amines	生物胺类
232	Spermidine	亚精胺	Spd	124-20-9	C7H19N3	1102	HMDB0001257	C00315	Biogenic Amines	生物胺类

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233	Acetylcholine	乙酰胆碱	Ach	51-84-3	C7H16NO2+	187	HMDB0000895	C01996	Biogenic Amines	生物胺类
234	Histamine	组胺	Hist	51-45-6	C5H9N3	774	HMDB0000870	C00388	Biogenic Amines	生物胺类
235	1,3-Diaminopropane	1,3-二氨基丙烷	/	109-76-2	C3H10N2	428	HMDB0000002	C00986	Biogenic Amines	生物胺类
236	Dopamine	多巴胺	DA	51-61-6	C8H11NO2	681	HMDB0000073	C03758	Biogenic Amines	生物胺类
237	Tryptamine	色胺	TRA	61-54-1	C10H12N2	1150	HMDB0000303	C00398	Biogenic Amines	生物胺类
238	Hordenine	大麦芽碱	/	539-15-1	C10H15NO	68313	HMDB0004366	C06199	Biogenic Amines	生物胺类
239	3-Methoxytyramine	3-甲氧酪胺	/	554-52-9	C9H13NO2	1669	HMDB0000022	C05587	Biogenic Amines	生物胺类
240	5-Methoxytryptamine	5-甲氧基色胺	/	608-07-1	C11H14N2O	1833	HMDB0004095	C05659	Biogenic Amines	生物胺类
241	Spermine	精胺	Spm	71-44-3	C10H26N4	1103	HMDB0001256	C00750	Biogenic Amines	生物胺类
242	N1-Acetylspermine	N1-乙酰精胺	/	25593-72-0	C12H28N4O	916	HMDB0001186	C02567	Biogenic Amines	生物胺类
243	N-Acetyl-5-hydroxytryptamine	N-乙酰-5-羟色胺	NAS	1210-83-9	C12H14N2O2	903	HMDB0001238	C00978	Biogenic Amines	生物胺类
244	Trimethylamine	三甲胺	TMA	75-50-3	C3H9N	1146	HMDB0000906	C00565	Biogenic Amines	生物胺类
245	Trimethylamine N-oxide	氧化三甲胺	TMAO	1184-78-7	C3H9NO	1145	HMDB0000925	C01104	Biogenic Amines	生物胺类
246	Diethanolamine	二乙醇胺	/	111-42-2	C4H11NO2	8113	HMDB0004437	C06772	Biogenic Amines	生物胺类
247	N-Acetylcadaverine	N-乙酰尸胺	/	32343-73-0	C7H16N2O	189087	HMDB0002284	/	Biogenic Amines	生物胺类
248	Tyramine	酪胺	TyrA	51-67-2	C8H11NO	5610	HMDB0000306	C00483	Biogenic Amines	生物胺类
249	Octopamine	章鱼胺	OA	104-14-3	C8H11NO2	4581	HMDB0004825	C04227	Biogenic Amines	生物胺类
250	Norepinephrine	去甲肾上腺素	NE	51-41-2	C8H11NO3	439260	HMDB0000216	C00547	Biogenic Amines	生物胺类
251	Epinephrine	肾上腺素	E	51-43-4	C9H13NO3	5816	HMDB0000068	C00788	Biogenic Amines	生物胺类
252	Histidinol	组氨醇	/	4836-52-6	C6H11N3O	165271	HMDB0003431	C00860	Biogenic Amines	生物胺类
253	4-Butyrobetaine	丁基甜菜碱	/	407-64-7	C7H15NO2	725	HMDB0001161	C01181	Biogenic Amines	生物胺类
254	Phosphorylcholine chloride	磷酸胆碱	/	3616-04-4	C5H15NO4P+	1014	HMDB0001565	C00588	Biogenic Amines	生物胺类
255	N-Methyltyramine	N-甲基酪胺	/	370-98-9	C9H13NO	9727	HMDB0003633	C02442	Biogenic Amines	生物胺类
256	Dimethylamine	二甲胺	/	124-40-3	C2H7N	674	HMDB0000087	C00543	Biogenic Amines	生物胺类

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257	Bis(3-Aminopropyl)Amine	双(3-氨基丙基)胺	/	56-18-8	C6H17N3	5942	HMDB0011634	C03375	Biogenic Amines	生物胺类
258	N-Acetylhistamine	N-乙酰组胺	/	673-49-4	C7H11N3O	69602	HMDB0013253	C05135	Biogenic Amines	生物胺类
259	3-Methylhistamine	3-甲基组胺	/	644-42-8	C6H11N3	69520	HMDB0001861	/	Biogenic Amines	生物胺类
260	Inositol	肌醇	/	87-89-8	C6H12O6	892	HMDB0000211	C00137	Carbohydrates	碳水化合物
261	Gluconic acid	葡萄糖酸	Gluconic acid	526-95-4	C6H12O7	10690	HMDB0000625	C00257	Carbohydrates	碳水化合物
262	Glucaric acid	葡萄糖二酸	/	87-73-0	C6H10O8	33037	HMDB0000663	C00818	Carbohydrates	碳水化合物
263	Ribose-5-Phosphate	核糖-5-磷酸	R5P	4300-28-1	C5H11O8P	77982	HMDB0001548	C00117	Carbohydrates	碳水化合物
264	Fructose-6-phosphate	果糖-6-磷酸	F6P	643-13-0	C6H13O9P	69507	HMDB0000124	C00085	Carbohydrates	碳水化合物
265	6-Phosphogluconic acid	6-磷酸葡萄糖酸	6PG	921-62-0	C6H13O10P	91493	HMDB0001316	C00345	Carbohydrates	碳水化合物
266	Sedoheptulose 7-phosphate	景天庚酮糖-7-磷酸	S7P	2646-35-7	C7H15O10P	165007	HMDB0258206	C05382	Carbohydrates	碳水化合物
267	Adenosine diphosphate glucose	ADP-葡萄糖	/	2140-58-1	C16H25N5O15P2	16500	HMDB0006557	C00498	Carbohydrates	碳水化合物
268	Erythritol	赤藓醇	/	149-32-6	C4H10O4	222285	HMDB0002994	C00503	Carbohydrates	碳水化合物
269	Glucosamine	氨基葡萄糖	GA	3416-24-8	C6H13NO5	439213	HMDB0001514	C00329	Carbohydrates	碳水化合物
270	D-Glucuronic acid	D-葡萄糖醛酸	/	528-16-5	C6H10O7	94715	HMDB0000127	C00191	Carbohydrates	碳水化合物
271	N-Acetyl-Glucosamine	N-乙酰葡糖胺	/	7512-17-6	C8H15NO6	439174	HMDB0000215	C00140	Carbohydrates	碳水化合物
272	Glucosamine 6-phosphate	氨基葡糖-6-磷酸	GlcN6P	3616-42-0	C6H14NO8P	440997	HMDB0001254	C00352	Carbohydrates	碳水化合物
273	Guanosine Diphosphate-Mannose	GDP-甘露糖	GDP-Man	3123-67-9	C16H25N5O16P2	135398627	HMDB0001163	C00096	Carbohydrates	碳水化合物
274	UDP-N-acetylglucosamine	UDP-N-乙酰氨基葡糖	UDP-NAG	528-04-1	C17H27N3O17P2	445675	HMDB0000290	C00043	Carbohydrates	碳水化合物
275	Dihydroxyacetone phosphate	二羟丙酮磷酸	/	57-04-5	C3H7O6P	668	HMDB0001473	C00111	Carbohydrates	碳水化合物
276	2-Phosphoglyceric acid	2-磷酸甘油酸	2PG	2553-59-5	C3H7O7P	59	HMDB0000362	/	Carbohydrates	碳水化合物
277	Threonic acid	苏糖酸	/	7306-96-9	C4H8O5	5460407	HMDB0000943	C01620	Carbohydrates	碳水化合物
278	Ribulose 1,5-bisphosphate	核酮糖-1,5-二磷酸	RuBP	24218-00-6	C5H12O11P2	123658	HMDB0304322	C01182	Carbohydrates	碳水化合物
279	Mannose 6-phosphate	甘露糖-6-磷酸	M6P	3672-15-9	C6H13O9P	65127	HMDB0304312	C00275	Carbohydrates	碳水化合物
280	Mannitol	甘露醇	/	69-65-8	C6H14O6	6251	HMDB0000765	C00392	Carbohydrates	碳水化合物

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281	D-Sorbitol	D-山梨醇	/	50-70-4	C6H14O6	5780	HMDB0000247	C00794	Carbohydrates	碳水化合物
282	Galactitol	半乳糖醇	/	608-66-2	C6H14O6	11850	HMDB0000107	C01697	Carbohydrates	碳水化合物
283	Glyceric acid	甘油酸	Glyceric acid	473-81-4	C3H6O4	752	HMDB0000139	C00258	Carbohydrates	碳水化合物
284	N-Acetyl-Neuraminic Acid	N-乙酰神经氨酸	/	131-48-6	C11H19NO9	445063	HMDB0000230	C19910	Carbohydrates	碳水化合物
285	Mannosamine	甘露糖胺	/	2636-92-2	C6H13NO5	440049	HMDB0250773	C03570	Carbohydrates	碳水化合物
286	Glucosamine-6-sulfate	氨基葡萄糖-6-硫酸	/	91674-26-9	C6H13NO8S	72361	HMDB0000592	/	Carbohydrates	碳水化合物
287	Trehalose-6-phosphate	海藻糖-6-磷酸	Tre6P	4484-88-2	C12H23O14P	122336	HMDB0001124	C00689	Carbohydrates	碳水化合物
288	1,5-Anhydroglucitol	1,5-脱水葡萄糖醇	/	154-58-5	C6H12O5	64960	HMDB0002712	C07326	Carbohydrates	碳水化合物
289	Ribonic acid	核糖酸	/	642-98-8	C5H10O6	5460677	HMDB0000867	C01685	Carbohydrates	碳水化合物
290	N-Acetyl-Muramic Acid	N-乙酰胞壁酸	/	2245794-62-9	C11H19NO8	5462244	HMDB0060493	C02713	Carbohydrates	碳水化合物
291	Erythronic Acid	赤藓糖酸	/	13752-84-6	C4H8O5	2781043	HMDB0000613	C21593	Carbohydrates	碳水化合物
292	Indoxyl Glucuronide	吲哚酚葡萄糖醛酸苷	/	35804-66-1	C14H15NO7	2733785	HMDB0010319	/	Carbohydrates	碳水化合物
293	Dopamine Glucuronide	多巴胺葡萄糖醛酸苷	/	38632-24-5	C14H19NO8	3082490	HMDB0010329	/	Carbohydrates	碳水化合物
294	Glycerophosphoric acid	3-磷酸甘油酸	/	57-03-4	C3H9O6P	754	HMDB0252849	C00093	Carbohydrates	碳水化合物
295	Sucrose	蔗糖	/	57-50-1	C12H22O11	5988	HMDB0000258	C00089	Sugars	糖类
296	D-Fructose	D-果糖	Fructose	57-48-7	C6H12O6	2723872	HMDB0000660	C00095	Sugars	糖类
297	Melibiose	蜜二糖	/	585-99-9	C12H22O11	440658	HMDB0000048	C05402	Sugars	糖类
298	Cellobiose	纤维二糖	/	528-50-7	C12H22O11	10712	HMDB0000055	C00185	Sugars	糖类
299	Stachyose	水苏糖	/	470-55-3	C24H42O21	439531	HMDB0003553	C01613	Sugars	糖类
300	Acarbose	阿卡波糖	/	56180-94-0	C25H43NO18	441184	HMDB0014429	C06802	Sugars	糖类
301	Xylose	木糖	/	58-86-6	C5H10O5	135191	HMDB0000098	C00181	Sugars	糖类
302	D-Ribose	核糖	/	50-69-1	C5H10O5	10975657	HMDB0000283	C00121	Sugars	糖类
303	L-Rhamnose	L-鼠李糖	/	3615-41-6	C6H12O5	25310	HMDB0000849	C00507	Sugars	糖类
304	D-Glucose	D-葡萄糖	D-Glucose	54-17-1	C6H12O6	5793	HMDB0000122	C00031	Sugars	糖类

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305	Lyxose	来苏糖	/	10257-34-8	C5H10O5	439240	/	C00476	Sugars	糖类
306	Pyridoxal	吡哆醛	/	66-72-8	C8H9NO3	1050	HMDB0001545	C00250	Vitamins	维生素类
307	Nicotinamide	烟酰胺	NAM	98-92-0	C6H6N2O	936	HMDB0001406	C00153	Vitamins	维生素类
308	Pyridoxamine	吡哆胺	/	85-87-0	C8H12N2O2	1052	HMDB0001431	C00534	Vitamins	维生素类
309	Pyridoxine	吡哆醇	/	65-23-6	C8H11NO3	1054	HMDB0000239	C00314	Vitamins	维生素类
310	Thiamine	维生素 B_1	/	70-16-6	C12H17N4OS+	1130	HMDB0000235	C00378	Vitamins	维生素类
311	Riboflavine	核黄素	/	83-88-5	C17H20N4O6	493570	HMDB0000244	C00255	Vitamins	维生素类
312	Pantothenic acid	维生素 B_5	/	79-83-4	C9H17NO5	6613	HMDB0000210	C00864	Vitamins	维生素类
313	Nicotinic acid	烟酸	NA	59-67-6	C6H5NO2	938	HMDB0001488	C00253	Vitamins	维生素类
314	Ascorbic Acid	抗坏血酸	/	50-81-7	C6H8O6	54670067	HMDB0000044	C00072	Vitamins	维生素类
315	alpha-Tocopherol (Vitamin E)	α-生育酚	/	59-02-9	C29H50O2	14985	HMDB0001893	C02477	Vitamins	维生素类
316	Cyanocobalamin	氰钴胺	/	68-19-9	C63H88CoN14O14P	5311498	HMDB0000607	C02823	Vitamins	维生素类
317	Thioctic acid	硫辛酸	/	1200-22-2	C8H14O2S2	6112	HMDB0001451	C16241	Vitamins	维生素类
318	Indole	吲哚	Indole	120-72-9	C8H7N	798	HMDB0000738	C00463	Indoles	吲哚类
319	Indole-3-acrylic acid	吲哚-3-丙烯酸	IA	1204-06-4	C11H9NO2	5375048	HMDB0000734	C21283	Indoles	吲哚类
320	Indole-3-carboxylic acid	吲哚-3-甲酸	ICA	771-50-6	C9H7NO2	69867	HMDB0003320	C19837	Indoles	吲哚类
321	N-Methyltryptamine	N-甲基色胺	/	61-49-4	C11H14N2	6088	HMDB0004370	C06213	Indoles	吲哚类
322	Serotonin	5-羟色胺/血清素	5-HT	50-67-9	C10H12N2O	5202	HMDB0000259	C00780	Indoles	吲哚类
323	5-Hydroxyindole-3-acetic acid	5-羟基吲哚-3-乙酸	5-HIAA	54-16-0	C10H9NO3	1826	HMDB0000763	C05635	Indoles	吲哚类
324	Melatonin	褪黑素	MT	73-31-4	C13H16N2O2	896	HMDB0001389	C01598	Indoles	吲哚类
325	6-Hydroxymelatonin	6-羟基褪黑素	/	2208-415	C13H16N2O3	1864	HMDB0004081	C05643	Indoles	吲哚类
326	Indole-3-acetamide	吲哚-3-乙酰胺	IAM	879-37-8	C10H10N2O	397	HMDB0029739	C02693	Indoles	吲哚类
327	Tryptophol	色醇	IE	526-55-6	C10H11NO	10685	HMDB0003447	C00955	Indoles	吲哚类

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328	5-Hydroxytryptophol	5-羟基色醇	5-HTOL	154-02-9	C10H11NO2	9061	HMDB0001855	/	Indoles	吲哚类
329	Indole-3-glyoxylic acid	吲哚-3-乙醛酸	IGA	1477-49-2	C10H7NO3	73863	HMDB0242143	/	Indoles	吲哚类
330	Indole-3-acetonitrile	吲哚-3-乙腈	IAN	771-51-7	C10H8N2	351795	HMDB0006524	C02938	Indoles	吲哚类
331	Indole-3-acetic acid	吲哚-3-乙酸	IAA	87-51-4	C10H9NO2	802	HMDB0000197	C00954	Indoles	吲哚类
332	Indole-3-methyl acetate	吲哚-3-乙酸甲酯	/	1912-33-0	C11H11NO2	74706	HMDB0029738	C20635	Indoles	吲哚类
333	Indole-3-propionic acid	吲哚-3-丙酸	IPA	830-96-6	C11H11NO2	3744	HMDB0002302	C22236	Indoles	吲哚类
334	5-Methoxyindole-3-acetic acid	5-甲氧基吲哚-3-乙酸	5-Me-IAA	3471-31-6	C11H11NO3	18986	HMDB0004096	C05660	Indoles	吲哚类
335	L-Tryptophan	L-色氨酸	Trp	73-22-3	C11H12N2O2	6305	HMDB0000929	C00078	Indoles	吲哚类
336	Indole-3-pyruvic acid	吲哚-3-丙酮酸	/	392-12-1	C11H9NO3	803	HMDB0060484	C00331	Indoles	吲哚类
337	Indole-3-butyric acid	吲哚-3-丁酸	IBA	133-32-4	C12H13NO2	8617	HMDB0002096	C11284	Indoles	吲哚类
338	Indoxyl-beta-D-glucoside	尿蓝母	Indican	487-60-5	C14H17NO6	441564	HMDB0061755	C08481	Indoles	吲哚类
339	Indoxylsulfate	硫酸吲哚酚	IS	487-94-5	C8H7NO4S	10258	HMDB0000682	/	Indoles	吲哚类
340	Indole-3-carboxaldehyde	吲哚-3-甲醛	ICAld	487-89-8	C9H7NO	10256	HMDB0029737	C08493	Indoles	吲哚类
341	Skatole	粪臭素	skatole	83-34-1	C9H9N	6736	HMDB0000466	C08313	Indoles	吲哚类
342	Indole-3-lactic acid	吲哚-3-乳酸	ILA	1821-52-9	C11H11NO3	92904	HMDB0000671	C02043	Indoles	吲哚类
343	5-Hydroxyindole	5-羟基吲哚	/	1953-54-4	C8H7NO	16054	HMDB0059805	/	Indoles	吲哚类
344	Indole-2-carboxylic acid	吲哚-2-甲酸	/	1477-50-5	C9H7NO2	72899	HMDB0002285	/	Indoles	吲哚类
345	3-Methyldioxyindole	3-甲基二氧吲哚	/	3040-34-4	C9H9NO2	151066	HMDB0004186	C05834	Indoles	吲哚类
346	N-methylserotonin	N-甲基羟色胺	/	1134-01-6	C11H14N2O	150885	HMDB0004369	C06212	Indoles	吲哚类
347	Indole-3-acetyl-L-alanine	吲哚-3-乙酰-L-丙氨酸	IAA-Ala	57105-39-2	C13H14N2O3	644225	/	/	Indoles	吲哚类
348	Indole-3-acetyl-L-aspartic acid	吲哚-3-乙酰-L-天冬氨酸	IAA-Asp	2456-73-7	C14H14N2O5	446620	HMDB0038666	C22224	Indoles	吲哚类
349	Indole-3-acetyl-glycine	吲哚-3-乙酰-甘氨酸	IAA-Gly	13113-08-1	C12H12N2O3	446640	HMDB0240661	/	Indoles	吲哚类
350	Glycolic Acid	乙醇酸	GL	79-14-1	C2H4O3	757	HMDB0000115	C00160	Organic acids	有机酸
351	Pyruvic acid	丙酮酸	PYR	127-17-3	C3H4O3	1060	HMDB0000243	C00022	Organic acids	有机酸

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352	L-Lactic acid	乳酸	Lac	79-33-4	C3H6O3	107689	HMDB0000190	C00186	Organic acids	有机酸
353	Fumaric acid	富马酸	FA	110-17-8	C4H4O4	444972	HMDB0000134	C00122	Organic acids	有机酸
354	Succinic acid	琥珀酸	Succinic acid	110-15-6	C4H6O4	1110	HMDB0000254	C00042	Organic acids	有机酸
355	Methylmalonic acid	甲基丙二酸/异琥珀酸	MMA	516-05-2	C4H6O4	487	HMDB0000202	C02170	Organic acids	有机酸
356	Taurine	牛磺酸	/	107-35-7	C2H7NO3S	1123	HMDB0000251	C00245	Organic acids	有机酸
357	Malic acid	苹果酸	MA	97-67-6	C4H6O5	222656	HMDB0000156	C00149	Organic acids	有机酸
358	alpha-Ketoglutaric acid	α-酮戊二酸	AKG	328-50-7	C5H6O5	51	HMDB0000208	C00026	Organic acids	有机酸
359	Phosphoenolpyruvic acid	磷酸烯醇式丙酮酸	PEP	138-08-9	C3H5O6P	1005	HMDB0000263	C00074	Organic acids	有机酸
360	Shikimic acid	莽草酸	/	138-59-0	C7H10O5	8742	HMDB0003070	C00493	Organic acids	有机酸
361	cis-Aconitic acid	顺式乌头酸	CAA	585-84-2	C6H6O6	643757	HMDB0000072	C00417	Organic acids	有机酸
362	Kynurenic acid	犬尿喹啉酸	KYNA	492-27-3	C10H7NO3	3845	HMDB0000715	C01717	Organic acids	有机酸
363	Isocitric acid	异柠檬酸	ICA	320-77-4	C6H8O7	1198	HMDB0000193	C00311	Organic acids	有机酸
364	Citric acid	柠檬酸	CA	77-92-9	C6H8O7	311	HMDB0000094	C00158	Organic acids	有机酸
365	2-Hydroxyglutaric acid	2-羟基戊二酸	2HG	2889-31-8	C5H8O5	43	HMDB0059655	C02630	Organic acids	有机酸
366	3-Hydroxybutyric acid	3-羟基丁酸	3HB	300-85-6	C4H8O3	441	HMDB0000011	C01089	Organic acids	有机酸
367	2-Oxobutanoic acid	2-酮丁酸	/	600-18-0	C4H6O3	58	HMDB0000005	C00109	Organic acids	有机酸
368	Acetoacetic acid	乙酰乙酸	/	541-50-4	C4H6O3	96	HMDB0000060	C00164	Organic acids	有机酸
369	Malonic acid	丙二酸	/	141-82-2	C3H4O4	867	HMDB0000691	C04025	Organic acids	有机酸
370	Hypotaurine	亚牛磺酸	/	300-84-5	C2H7NO2S	107812	HMDB0000965	C00519	Organic acids	有机酸
371	Maleic acid	马来酸/顺丁烯二酸	Maleic acid	110-16-7	C4H4O4	444266	HMDB0000176	C01384	Organic acids	有机酸
372	Benzoic acid	苯甲酸	/	65-85-0	C7H6O2	243	HMDB0001870	C00180	Organic acids	有机酸
373	2-Oxohexanoic acid	2-氧代己酸	/	2492-75-3	C6H10O3	159664	HMDB0001864	C00902	Organic acids	有机酸
374	3-Methyl-2-oxovaleric acid	3-甲基-2-氧基戊酸	/	24809-08-3	C6H10O3	47	HMDB0000491	C00671	Organic acids	有机酸
375	Acetyl Phosphate	乙酰磷酸	/	590-54-5	C2H5O5P	186	HMDB0001494	C00227	Organic acids	有机酸

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376	Adipic acid	己二酸	/	124-04-9	C6H10O4	196	HMDB0000448	C06104	Organic acids	有机酸
377	Citramalic acid	柠苹酸	/	597-44-4	C5H8O5	1081	HMDB0000426	C00815	Organic acids	有机酸
378	Mevalonic acid	甲羟戊酸	MVA	17817-88-8	C6H12O4	449	HMDB0000227	C00418	Organic acids	有机酸
379	Tartaric acid	酒石酸	/	87-69-4	C4H6O6	444305	HMDB0000956	C00898	Organic acids	有机酸
380	Gentisic acid	龙胆酸	/	490-79-9	C7H6O4	3469	HMDB0000152	C00628	Organic acids	有机酸
381	2-Oxoadipic acid	α-酮己二酸	Oxoadipic acid	3184-35-8	C6H8O5	71	HMDB0000225	C00322	Organic acids	有机酸
382	Pimelic acid	庚二酸	/	111-16-0	C7H12O4	385	HMDB0000857	C02656	Organic acids	有机酸
383	3-Hydroxy-3-methylglutaric acid	3-羟基-3-甲基戊二酸	/	503-49-1	C6H10O5	1662	HMDB0000355	C03761	Organic acids	有机酸
384	Homogentisic acid	尿黑酸	HGA	451-13-8	C8H8O4	780	HMDB0000130	C00544	Organic acids	有机酸
385	Vanillic acid	香草酸	/	121-34-6	C8H8O4	8468	HMDB0000484	C06672	Organic acids	有机酸
386	2-Isopropylmalic acid	2-异丙基苹果酸	/	49601-06-1	C7H12O5	5280523	HMDB0000402	C02504	Organic acids	有机酸
387	Azelaic acid	壬二酸	/	123-99-9	C9H16O4	2266	HMDB0000784	C08261	Organic acids	有机酸
388	Isoferulic acid	异阿魏酸	/	25522-33-2	C10H10O4	736186	HMDB0000955	C10470	Organic acids	有机酸
389	Ferulate	阿魏酸	/	537-98-4	C10H10O4	445858	HMDB0000954	C01494	Organic acids	有机酸
390	Sebacic acid	癸二酸	/	111-20-6	C10H18O4	5192	HMDB0000792	C08277	Organic acids	有机酸
391	Oxalic acid	草酸	/	144-62-7	C2H2O4	971	HMDB0002329	C00209	Organic acids	有机酸
392	O-Phosphoethanolamine	磷酸乙醇胺	/	1071-23-4	C2H8NO4P	1015	HMDB0000224	C00346	Organic acids	有机酸
393	3-Hydroxypropionic acid	3-羟基丙酸	3-HP	503-66-2	C3H6O3	68152	HMDB0000700	C01013	Organic acids	有机酸
394	1-Aminocyclopropanecarboxylic acid	1-氨基环丙烷羧酸	ACC	22059-21-8	C4H7NO2	535	HMDB0036458	C01234	Organic acids	有机酸
395	3-Ureidopropionic acid	3-脲基丙酸	/	462-88-4	C4H8N2O3	111	HMDB0000026	C02642	Organic acids	有机酸
396	3-Hydroxyisobutyric acid	3-羟基异丁酸	/	2068-83-9	C4H8O3	87	HMDB0000023	C06001	Organic acids	有机酸
397	2-Hydroxybutyric acid	2-羟基丁酸	2HB	600-15-7	C4H8O3	11266	HMDB0000008	C05984	Organic acids	有机酸
398	beta-Hydroxyisovaleric acid	β-羟基异戊酸	/	625-08-1	C5H10O3	69362	HMDB0000754	C20827	Organic acids	有机酸
399	Citraconic acid	柠康酸	/	498-23-7	C5H6O4	643798	HMDB0000634	C02226	Organic acids	有机酸

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400	Itaconic acid	衣康酸	IA	97-65-4	C5H6O4	811	HMDB0002092	C00490	Organic acids	有机酸
401	Glutaric acid	戊二酸	/	110-94-1	C5H8O4	743	HMDB0000661	C00489	Organic acids	有机酸
402	4-Methyl-2-oxopentanoic acid	4-甲基-2-氧戊酸	/	816-66-0	C6H10O3	70	HMDB0000695	C00233	Organic acids	有机酸
403	L-Pipecolic acid	L-2-哌啶酸	/	3105-95-1	C6H11NO2	439227	HMDB0000716	C00408	Organic acids	有机酸
404	2-Hydroxyisocaproic acid	2-羟基-4-甲基戊酸	/	13748-90-8	C6H12O3	83697	HMDB0000746	/	Organic acids	有机酸
405	Imidazolepropionic acid	咪唑丙酸	/	1074-59-5	C6H8N2O2	70630	HMDB0002271	C20522	Organic acids	有机酸
406	4,6-Dioxoheptanoic Acid	4,6-二氧庚酸	/	51568-18-4	C7H10O4	5312	HMDB0000635	/	Organic acids	有机酸
407	Salicylic acid	水杨酸	SA	69-72-7	C7H6O3	338	HMDB0001895	C00805	Organic acids	有机酸
408	Protocatechuic acid	原儿茶酸	/	99-50-3	C7H6O4	72	HMDB0001856	C00230	Organic acids	有机酸
409	Suberic acid	辛二酸	/	505-48-6	C8H14O4	10457	HMDB0000893	C08278	Organic acids	有机酸
410	Tranexamic Acid	氨甲环酸	/	1197-18-8	C8H15NO2	5526	/	/	Organic acids	有机酸
411	Phenylacetic acid	苯乙酸	/	103-82-2	C8H8O2	999	HMDB0000209	C07086	Organic acids	有机酸
412	3-Phenylpropionic acid	3-苯丙酸	/	501-52-0	C9H10O2	107	HMDB0000764	C05629	Organic acids	有机酸
413	Homovanillic acid	高香草酸	HVA	306-08-1	C9H10O4	1738	HMDB0000118	C05582	Organic acids	有机酸
414	Syringic acid	丁香酸	/	530-57-4	C9H10O5	10742	HMDB0002085	C10833	Organic acids	有机酸
415	Vanillylmandelic acid	香草扁桃酸	VMA	55-10-7	C9H10O5	1245	HMDB0000291	C05584	Organic acids	有机酸
416	trans-Cinnamic acid	反式肉桂酸	/	140-10-3	C9H8O2	444539	HMDB0000930	C00423	Organic acids	有机酸
417	2-Hydroxycinnamic acid	2-羟基肉桂酸	/	614-60-8	C9H8O3	637540	HMDB0002641	C01772	Organic acids	有机酸
418	Caffeic acid	咖啡酸	/	331-39-5	C9H8O4	689043	HMDB0001964	C01481	Organic acids	有机酸
419	2-Methylhexanoic Acid	2-甲基己酸	/	4536-23-6	C7H14O2	20653	HMDB0031594	/	Organic acids	有机酸
420	3-Hydroxydecanoic acid	3-羟基癸酸	/	14292-26-3	C10H20O3	26612	HMDB0002203	/	Organic acids	有机酸
421	2-Hydroxy-2-methylbutyric acid	2-羟基-2-甲基正丁酸	/	3739-30-8	C5H10O3	95433	HMDB0001987	/	Organic acids	有机酸
422	2-Hydroxy-3-methylbutyric acid	2-羟基-3-甲基丁酸	/	4026-18-0	C5H10O3	99823	HMDB0000407	/	Organic acids	有机酸
423	3-Guanidinopropionic acid	3-胍基丙酸	/	353-09-3	C4H9N3O2	67701	HMDB0013222	C03065	Organic acids	有机酸

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424	2-Methylsuccinic acid	2-甲基琥珀酸	/	498-21-5	C5H8O4	10349	HMDB0001844	C08645	Organic acids	有机酸
425	3-Hydroxyglutaric acid	3-羟基戊二酸	/	638-18-6	C5H8O5	181976	HMDB0000428	/	Organic acids	有机酸
426	N-Isovaleroylglycine	N-异戊酰氨基乙酸	/	16284-60-9	C7H13NO3	546304	HMDB0000678	/	Organic acids	有机酸
427	Isethionic Acid	羟乙磺酸	/	107-36-8	C2H6O4S	7866	HMDB0003903	C05123	Organic acids	有机酸
428	Tiglic acid	惕格酸	/	80-59-1	C5H8O2	125468	HMDB0001470	C08279	Organic acids	有机酸
429	2-Methylglutaric acid	2-甲基戊二酸	/	617-62-9	C6H10O4	12046	HMDB0000422	C02930	Organic acids	有机酸
430	3-Methyladipic acid	3-甲基己二酸	/	3058-01-3	C7H12O4	12292	HMDB0000555	/	Organic acids	有机酸
431	2-Hydroxyadipic acid	2-羟基己二酸	/	18294-85-4	C6H10O5	193530	HMDB0000321	C02360	Organic acids	有机酸
432	Atrolactic acid	苯乳酸	/	515-30-0	C9H10O3	1303	HMDB0000779	/	Organic acids	有机酸
433	Quinic acid	奎尼酸	/	77-95-2	C7H12O6	6508	HMDB0003072	C00296	Organic acids	有机酸
434	2-Methylcitric acid	2-甲基柠檬酸	/	6061-96-7	C7H10O7	515	HMDB0000379	C02225	Organic acids	有机酸
435	Ethylmalonic acid	乙基丙二酸	/	601-75-2	C5H8O4	11756	HMDB0000622	/	Organic acids	有机酸
436	2-Hydroxydecanoate	2-羟基癸酸	/	5393-81-7	C10H20O3	21488	HMDB0242148	/	Organic acids	有机酸
437	Levulinic acid	乙酰丙酸	/	123-76-2	C5H8O3	11579	HMDB0000720	/	Organic acids	有机酸
438	Furoic acid	糠酸	/	88-14-2	C5H4O3	6919	HMDB0000617	C01546	Organic acids	有机酸
439	Cyclohexylcarboxylic Acid	环己基羧酸	/	98-89-5	C7H12O2	7413	HMDB0031342	C09822	Organic acids	有机酸
440	3-Methylsalicylic acid	3-甲基水杨酸	/	83-40-9	C8H8O3	6738	HMDB0002390	C14088	Organic acids	有机酸
441	Mandelic acid	扁桃酸	/	90-64-2	C8H8O3	439616	HMDB0000703	C01984	Organic acids	有机酸
442	Diaminopimelic acid	二氨基庚二酸	/	583-93-7	C7H14N2O4	865	HMDB0242532	C00666	Organic acids	有机酸
443	3-Furoic acid	3-呋喃甲酸	/	488-93-7	C5H4O3	10268	HMDB0000444	/	Organic acids	有机酸
444	Senecioate	千里光酸	/	541-47-9	C5H8O2	10931	HMDB0000509	/	Organic acids	有机酸
445	Crotonic Acid	巴豆酸	/	107-93-7	C4H6O2	637090	HMDB0010720	C01771	Organic acids	有机酸
446	2-Phenylbutyric Acid	2-苯基丁酸	/	90-27-7	C10H12O2	7012	HMDB0000329	/	Organic acids	有机酸
447	8-Aminooctanoic Acid	8-氨基辛酸	/	27306-03-2	C8H17NO2	66085	HMDB0247418	/	Organic acids	有机酸

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448	Homoveratric acid	高藜芦酸	/	93-40-3	C10H12O4	7139	HMDB0000434	/	Organic acids	有机酸
449	Tricarballylic Acid	2-羧基戊二酸	/	99-14-9	C6H8O6	14925	HMDB0031193	C19806	Organic acids	有机酸
450	5-Phenylvaleric Acid	5-苯基戊酸	/	2270-20-4	C11H14O2	16757	HMDB0002043	/	Organic acids	有机酸
451	2-Phenylpropionic Acid	2-苯基丙酸	/	492-37-5	C9H10O2	10296	HMDB0011743	/	Organic acids	有机酸
452	3-O-Methylgallic Acid	3-O-甲基没食子酸	/	3934-84-7	C8H8O5	19829	/	C05616	Organic acids	有机酸
453	3-Phenylbutyric acid	3-苯基丁酸	/	4593-90-2	C10H12O2	20724	HMDB0001955	/	Organic acids	有机酸
454	2-Hydroxyoctanoic acid	2-羟基辛酸	/	617-73-2	C8H16O3	94180	HMDB0000711	/	Organic acids	有机酸
455	2-Hydroxy-4-(Methylthio)Butyric Acid	2-羟基-4-(甲硫基)丁酸	/	583-91-5	C5H10O3S	11427	HMDB0037115	/	Organic acids	有机酸
456	Omega-Hydroxydodecanoic Acid	ω-羟基十二烷酸	/	505-95-3	C12H24O3	79034	HMDB0002059	C08317	Organic acids	有机酸
457	Aminomalonic Acid	氨基丙二酸	/	1068-84-4	C3H5NO4	100714	HMDB0001147	C00872	Organic acids	有机酸
458	2-Hydroxycaproic acid	2-羟基己酸	/	6064-63-7	C6H12O3	99824	HMDB0001624	/	Organic acids	有机酸
459	4-Hydroxycyclohexylcarboxylic Acid	4-羟基环己基羧酸	/	17419-81-7	C7H12O3	151138	HMDB0001988	C04404	Organic acids	有机酸
460	3,4,5-Trimethoxycinnamic Acid	3,4,5-三甲氧基肉桂酸	/	20329-98-0	C12H14O5	735755	HMDB0002511	/	Organic acids	有机酸
461	3-Hydroxyoctanoic acid	3-羟基辛酸	/	14292-27-4	C8H16O3	26613	HMDB0001954	C20793	Organic acids	有机酸
462	3-Aminobenzoic acid	间氨基苯甲酸	/	99-05-8	C7H7NO2	7419	HMDB0001891	/	Organic acids	有机酸
463	3-Aminosalicylic acid	3-氨基水杨酸	/	570-23-0	C7H7NO3	68443	HMDB0001972	/	Organic acids	有机酸
464	3-Hydroxysebacic Acid	3-羟基癸二酸	/	73141-46-5	C10H18O5	3017884	HMDB0340579	/	Organic acids	有机酸
465	Argininic acid	(S)-5-胍基-2-羟基戊酸	/	157-07-3	C6H13N3O3	160437	HMDB0003148	/	Organic acids	有机酸
466	Phenylbutyric acid	苯丁酸	/	1821-12-1	C10H12O2	4775	HMDB0000543	C21793	Organic acids	有机酸
467	4-O-Methylgallic Acid	4-O-甲基没食子酸	/	4319-02-2	C8H8O5	78016	HMDB0013198	/	Organic acids	有机酸
468	Ferulic Acid-4-Sulfate	阿魏酸-4-硫酸	/	86321-29-1	C10H10O7S	6305574	HMDB0029200	/	Organic acids	有机酸
469	2-Methyl-3-hydroxybutyric acid	2-甲基-3-羟基丁酸	/	473-86-9	C5H10O3	160471	HMDB0000354	/	Organic acids	有机酸
470	4-Hydroxycyclohexylacetate	4-羟基环己基乙酸	/	99799-09-4	C8H14O3	12702257	HMDB0000451	/	Organic acids	有机酸
471	Cis-4-Octenedioate	顺式-4-辛烯二酸	/	38561-68-1	C8H12O4	11805205	HMDB0004982	/	Organic acids	有机酸

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472	2-Hydroxyvaleric Acid	2-羟基戊酸	/	617-31-2	C5H10O3	98009	HMDB0001863	/	Organic acids	有机酸
473	2-Ethyl-2-hydroxybutyric acid	2-乙基-2-羟基丁酸	/	3639-21-2	C6H12O3	77199	HMDB0001975	/	Organic acids	有机酸
474	3-Hydroxydodecanedioate	3-羟基十二烷二酸	/	34574-69-1	C12H22O5	16663321	HMDB0000413	/	Organic acids	有机酸
475	3-Hydroxysuberate	3-羟基辛二酸	/	73141-47-6	C8H14O5	22328017	HMDB0000325	/	Organic acids	有机酸
476	Valproic acid	丙戊酸	/	99-66-1	C8H16O2	3121	HMDB0001877	C07185	Fatty Acids	脂肪酸类
477	Adenosine	腺苷	ADO	58-61-7	C10H13N5O4	60961	HMDB0000050	C00212	Nucleosides	核苷类
478	S-Adenosylmethionine	S-腺苷甲硫氨酸	SAM	29908-03-0	C15H22N6O5S	34755	HMDB0001185	C00019	Nucleosides	核苷类
479	Nicotinamide adenine dinucleotid	烟酰胺腺嘌呤二核苷酸	NAD	53-84-9	C21H27N7O14P2	5892	HMDB0000902	C00003	Nucleosides	核苷类
480	1,4-Dihydronicotinamide adenine dinucleotide	还原型烟酰胺腺嘌呤二核苷酸	NADH	58-68-4	C21H29N7O14P2	439153	HMDB0001487	C00004	Nucleosides	核苷类
481	Flavin adenine dinucleotide	黄素腺嘌呤二核苷酸	FAD	146-14-5	C27H33N9O15P2	643975	HMDB0001248	C00016	Nucleosides	核苷类
482	Thymidine	胸苷	T	50-89-5	C10H14N2O5	5789	HMDB0000273	C00214	Nucleosides	核苷类
483	Uridine	尿苷	U	58-96-8	C9H12N2O6	6029	HMDB0000296	C00299	Nucleosides	核苷类
484	Inosine	肌苷	Ino	58-63-9	C10H12N4O5	135398641	HMDB0000195	C00294	Nucleosides	核苷类
485	Adenosine-5'-diphosphate	腺苷-5'-二磷酸	ADP	58-64-0	C10H15N5O10P2	6022	HMDB0001341	C00008	Nucleosides	核苷类
486	Flavin mononucleotide	黄素单核苷酸	FMN	146-17-8	C17H21N4O9P	643976	HMDB0001520	C00061	Nucleosides	核苷类
487	Adenosine-5'-triphosphate	腺苷-5'-三磷酸	ATP	56-65-5	C10H16N5O13P3	5957	HMDB0000538	C00002	Nucleosides	核苷类
488	Guanosine-5'-triphosphate	鸟苷-5'-三磷酸	GTP	86-01-1	C10H16N5O14P3	135398633	HMDB0001273	C00044	Nucleosides	核苷类
489	2'-Deoxyuridine	2'-脱氧尿苷	/	951-78-0	C9H12N2O5	13712	HMDB0000012	C00526	Nucleosides	核苷类
490	5'-Deoxyadenosine	5'-脱氧腺苷	/	4754-39-6	C10H13N5O3	439182	HMDB0001983	C05198	Nucleosides	核苷类
491	1-Methyladenosine	1-甲基腺苷	/	15763-06-1	C11H15N5O4	27476	HMDB0003331	C02494	Nucleosides	核苷类
492	Xanthosine	黄苷	/	146-80-5	C10H12N4O6	64959	HMDB0000299	C01762	Nucleosides	核苷类
493	2'-Deoxycytidine-5'-monophosphate	2'-脱氧胞苷-5'-单磷酸	dCMP	1032-65-1	C9H14N3O7P	13945	HMDB0001202	C00239	Nucleosides	核苷类
494	Deoxyuridine monophosphate	脱氧尿苷单磷酸	dUMP	964-26-1	C9H13N2O8P	65063	HMDB0001409	C00365	Nucleosides	核苷类

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495	Thymidine-5'-phosphate	胸苷-5'-单磷酸	TMP	365-07-1	C10H15N2O8P	9700	HMDB0001227	C00364	Nucleosides	核苷类
496	2'-Deoxyadenosine-5'-monophosphate	2′-脱氧腺苷-5′-单磷酸	dAMP	653-63-4	C10H14N5O6P	12599	HMDB0000905	C00360	Nucleosides	核苷类
497	2'-Deoxyguanosine-5'-monophosphate	2′-脱氧鸟苷-5′-单磷酸	dGMP	902-04-5	C10H14N5O7P	135398597	HMDB0001044	C00362	Nucleosides	核苷类
498	Adenosine-5'-Monophosphate	腺苷酸	AMP	61-19-8	C10H14N5O7P	6083	HMDB0000045	C00020	Nucleosides	核苷类
499	Xanthylic acid	黄苷-5'-单磷酸	XMP	523-98-8	C10H13N4O9P	73323	HMDB0001554	C00655	Nucleosides	核苷类
500	S-Adenosyl-homocysteine	S-腺苷-高半胱氨酸	SAH	979-92-0	C14H20N6O5S	439155	HMDB0000939	C00021	Nucleosides	核苷类
501	2'-Deoxycytidine-5'-diphosphate	2′-脱氧胞苷-5'-二磷酸	dCDP	800-73-7	C9H15N3O10P2	150855	HMDB0001245	C00705	Nucleosides	核苷类
502	Cytidine-5'-diphosphate	胞苷-5'-二磷酸	CDP	63-38-7	C9H15N3O11P2	6132	HMDB0001546	C00112	Nucleosides	核苷类
503	Uridine-5'-diphosphate	尿苷-5'-二磷酸	UDP	58-98-0	C9H14N2O12P2	6031	HMDB0000295	C00015	Nucleosides	核苷类
504	Adenosine-3'-5'-diphosphate	腺苷-3'-5'-二磷酸	/	1053-73-2	C10H15N5O10P2	159296	HMDB0000061	C00054	Nucleosides	核苷类
505	Inosine 5'-diphosphate	肌苷-5'-二磷酸	IDP	86-04-4	C10H14N4O11P2	135398651	HMDB0003335	C00104	Nucleosides	核苷类
506	Cytidine-5'-triphosphate	胞苷-5'-三磷酸	/	65-47-4	C9H16N3O14P3	6176	HMDB0000082	C00063	Nucleosides	核苷类
507	Uridine 5'-triphosphate	尿苷-5'-三磷酸	UTP	63-39-8	C9H15N2O15P3	6133	HMDB0000285	C00075	Nucleosides	核苷类
508	2'-Deoxyadenosine-5'-triphosphate	2'-脱氧腺苷-5'-三磷酸	/	1927-31-7	C10H16N5O12P3	15993	HMDB0001532	C00131	Nucleosides	核苷类
509	2'-Deoxyguanosine-5'-triphosphate	2'-脱氧鸟苷-5'-三磷酸	/	2564-35-4	C10H16N5O13P3	135398599	HMDB0001440	C00286	Nucleosides	核苷类
510	Uridine diphosphate glucuronic acid	UDP-葡萄糖醛酸	UDPGA	2616-64-0	C15H22N2O18P2	17473	HMDB0000935	C00167	Nucleosides	核苷类
511	3',5'-cyclic AMP	环腺苷酸	cAMP	60-92-4	C10H12N5O6P	6076	HMDB0000058	C00575	Nucleosides	核苷类
512	Inosinic acid	肌苷酸	IMP	131-99-7	C10H13N4O8P	135398640	HMDB0000175	C00130	Nucleosides	核苷类
513	8-Hydroxy-2'-deoxyguanosine	8-羟基-2'-脱氧鸟苷	/	88847-89-6	C10H13N5O5	73318	HMDB0003333	/	Nucleosides	核苷类
514	5-Methyluridine	5-甲基尿苷	/	1463-10-1	C10H14N2O6	445408	HMDB0000884	/	Nucleosides	核苷类
515	Guanosine-5'-Monophosphate	鸟苷酸	GMP	85-32-5	C10H14N5O8P	135398631	HMDB0001397	C00144	Nucleosides	核苷类
516	Guanosine-5'-diphosphate	鸟苷-5'-二磷酸	GDP	146-91-8	C10H15N5O11P2	135398619	HMDB0001201	C00035	Nucleosides	核苷类
517	Nicotinamide mononucleotide	烟酰胺单核苷酸	NMN	1094-61-7	C11H15N2O8P	14180	HMDB0000229	C00455	Nucleosides	核苷类
518	5'-Deoxy-5'-methylthioadenosine	5′-脱氧-5′-甲硫腺苷	/	2457-80-9	C11H15N5O3S	439176	HMDB0001173	C00170	Nucleosides	核苷类

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519	Cytidine 2',3'-cyclic phosphate	胞苷 2',3'-环磷酸	/	15718-51-1	C9H12N3O7P	53481030	HMDB0011691	C02354	Nucleosides	核苷类
520	Uridine-5'-monophosphate	尿苷-5'-单磷酸	UMP	58-97-9	C9H13N2O9P	6030	HMDB0000288	C00105	Nucleosides	核苷类
521	2'-Deoxycytidine	2'-脱氧胞苷	/	951-77-9	C9H13N3O4	13711	HMDB0000014	C00881	Nucleosides	核苷类
522	Cytidine	胞苷	C	65-46-3	C9H13N3O5	6175	HMDB0000089	C00475	Nucleosides	核苷类
523	Guanosine	鸟苷	G	118-00-3	C10H13N5O5	135398635	HMDB0000133	C00387	Nucleosides	核苷类
524	2'-Deoxyguanosine-5'-diphosphate	2'-脱氧鸟苷-5'-二磷酸	/	3493-09-2	C10H15N5O10P2	135398595	HMDB0000960	C00361	Nucleosides	核苷类
525	Pseudouridine	假尿苷	/	1445-07-4	C9H12N2O6	15047	HMDB0000767	C02067	Nucleosides	核苷类
526	3',5'-cyclic GMP	环磷酸鸟苷	cGMP	7665-99-8	C10H12N5O7P	135398570	HMDB0001314	C00942	Nucleosides	核苷类
527	1-Methylguanosine	1-甲基鸟苷	/	2140-65-0	C11H15N5O5	96373	HMDB0001563	C04545	Nucleosides	核苷类
528	2'-Deoxyadenosine-5'-diphosphate	2'-脱氧腺苷-5'-二磷酸	/	72003-83-9	C10H15N5O9P2	188966	HMDB0001508	C00206	Nucleosides	核苷类
529	Glucuronolactone	葡萄糖醛酸内酯	/	32449-92-6	C6H8O6	92283	/	C02670	Nucleosides	核苷类
530	7-Methylinosine	7-甲基肌苷	/	20245-33-4	C11H15N4O5+	135926583	/	/	Nucleosides	核苷类
531	Adenosine 2',3'-cyclic phosphate	腺苷 2',3'-环磷酸	/	634-01-5	C10H12N5O6P	101812	HMDB0011616	C02353	Nucleosides	核苷类
532	N6-Carbamoylthreonyladenosine	N6-氨甲酰苏氨酰腺苷	/	24719-82-2	C15H20N6O8	161466	/	/	Nucleosides	核苷类
533	3'-Cytidylic acid	3'-胞苷酸	/	84-52-6	C9H14N3O8P	66535	HMDB0240312	C05822	Nucleosides	核苷类
534	Estrone	雌酮	E1	53-16-7	C18H22O2	5870	HMDB0000145	C00468	Steroids	类固醇类
535	Estriol	雌三醇	E3	50-27-1	C18H24O3	5756	HMDB0000153	C05141	Steroids	类固醇类
536	Cortisone	皮质素/可的松	Cortisone	53-06-5	C21H28O5	222786	HMDB0002802	C00762	Steroids	类固醇类
537	Corticosterone	皮质酮	Cort	50-22-6	C21H30O4	5753	HMDB0001547	C02140	Steroids	类固醇类
538	Hydrocortisone	皮质醇/氢化可的松	F	50-23-7	C21H30O5	5754	HMDB0000063	C00735	Steroids	类固醇类
539	16-Dehydroprogesterone	16-脱氢孕酮	/	1096-38-4	C21H28O2	101964	HMDB0000995	C03207	Steroids	类固醇类
540	Cytosine	胞嘧啶	C	71-30-7	C4H5N3O	597	HMDB0000630	C00380	Pyrimidines	嘧啶类
541	Thymine	胸腺嘧啶	T	65-71-4	C5H6N2O2	1135	HMDB0000262	C00178	Pyrimidines	嘧啶类
542	Uracil	尿嘧啶	U	66-22-8	C4H4N2O2	1174	HMDB0000300	C00106	Pyrimidines	嘧啶类

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543	Dihydrothymine	二氢胸腺嘧啶	/	696-04-8	C5H8N2O2	93556	HMDB0304210	C00906	Pyrimidines	嘧啶类
544	5-Methylcytosine	5-甲基胞嘧啶	/	554-01-8	C5H7N3O	65040	HMDB0002894	C02376	Pyrimidines	嘧啶类
545	5-Hydroxymethyluracil	5-羟甲基尿嘧啶	/	4433-40-3	C5H6N2O3	78168	HMDB0000469	C03088	Pyrimidines	嘧啶类
546	Orotic acid	乳清酸	/	65-86-1	C5H4N2O4	967	HMDB0000226	C00295	Pyrimidines	嘧啶类
547	Thiamine monophosphate	单磷酸硫胺	/	495-23-8	C12H18N4O4PS+	3382778	HMDB0002666	C01081	Pyrimidines	嘧啶类
548	Ectoine	四氢嘧啶	/	96702-03-3	C6H10N2O2	126041	HMDB0240650	C06231	Pyrimidines	嘧啶类
549	2,4-Dihydroxypyrimidine-5-carboxylic acid	脲嘧啶-5-羧酸	/	23945-44-0	C5H4N2O4	90301	/	C03030	Pyrimidines	嘧啶类
550	Thiamine pyrophosphate	硫胺素焦磷酸	TPP	136-08-3	C12H19N4O7P2S+	1132	HMDB0001372	C00068	Pyrimidines	嘧啶类
551	1,3-Dimethyluracil	1,3-二甲基尿嘧啶	/	874-14-6	C6H8N2O2	70122	HMDB0002144	/	Pyrimidines	嘧啶类
552	Purine	嘌呤	/	120-73-0	C5H4N4	1044	HMDB0001366	C15587	Purines	嘌呤类
553	Adenine	腺嘌呤	A	73-24-5	C5H5N5	190	HMDB0000034	C00147	Purines	嘌呤类
554	Guanine	鸟嘌呤	G	73-40-5	C5H5N5O	135398634	HMDB0000132	C00242	Purines	嘌呤类
555	Hypoxanthine	次黄嘌呤	Hyp	68-94-0	C5H4N4O	135398638	HMDB0000157	C00262	Purines	嘌呤类
556	Xanthine	黄嘌呤	/	69-89-6	C5H4N4O2	1188	HMDB0000292	C00385	Purines	嘌呤类
557	Uric acid	尿酸	/	69-93-2	C5H4N4O3	1175	HMDB0000289	C00366	Purines	嘌呤类
558	1-Methylxanthine	1-甲基黄嘌呤	/	6136-37-4	C6H6N4O2	80220	HMDB0010738	C16358	Purines	嘌呤类
559	7-Methylxanthine	7-甲基黄嘌呤	/	552-62-5	C6H6N4O2	68374	HMDB0001991	C16353	Purines	嘌呤类
560	Paraxanthine	副黄嘌呤	/	611-59-6	C7H8N4O2	4687	HMDB0001860	C13747	Purines	嘌呤类
561	Theophylline	茶碱	/	58-55-9	C7H8N4O2	2153	HMDB0001889	C07130	Purines	嘌呤类
562	1-Methyluric acid	1-甲基尿酸	/	708-79-2	C6H6N4O3	69726	HMDB0003099	C16359	Purines	嘌呤类
563	1,7-Dimethyluric acid	1,7-二甲基尿酸	/	33868-03-0	C7H8N4O3	91611	HMDB0011103	C16356	Purines	嘌呤类
564	3-Methylxanthine	3-甲基黄嘌呤	/	1076-22-8	C6H6N4O2	70639	HMDB0001886	C16357	Purines	嘌呤类
565	1,3,7-Trimethyluric acid	1,3,7-三甲基尿酸	/	5415-44-1	C8H10N4O3	79437	HMDB0002123	C16361	Purines	嘌呤类
566	1,3-Dimethyluric-Acid	1,3-二甲基尿酸	/	944-73-0	C7H8N4O3	70346	HMDB0001857	/	Purines	嘌呤类

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567	3-Methyladenine	3-甲基腺嘌呤	/	5142-23-4	C6H7N5	135398661	HMDB0011600	C00913	Purines	嘌呤类
568	6,8-Dihydroxypurine	6,8-二羟基嘌呤	/	13231-00-0	C5H4N4O2	135414099	HMDB0001182	/	Purines	嘌呤类
569	1-Methylguanine	1-甲基鸟嘌呤	/	938-85-2	C6H7N5O	70315	HMDB0003282	C04152	Purines	嘌呤类
570	2-Aminobenzoic acid	邻氨基苯甲酸	AA	118-92-3	C7H7NO2	227	HMDB0001123	C00108	Benzenoids	苯类
571	4-Hydroxybenzoic acid	对羟基苯甲酸	/	99-96-7	C7H6O3	135	HMDB0000500	C00156	Benzenoids	苯类
572	p-Hydroxyphenylacetic acid	对羟基苯乙酸	/	156-38-7	C8H8O3	127	HMDB0000020	C00642	Benzenoids	苯类
573	Phenylpyruvic acid	苯丙酮酸	/	156-06-9	C9H8O3	997	HMDB0000205	C00166	Benzenoids	苯类
574	Phenol	苯酚	/	108-95-2	C6H6O	996	HMDB0000228	C00146	Benzenoids	苯类
575	4-Methylcatechol	4-甲基邻苯二酚	/	452-86-8	C7H8O2	9958	HMDB0000873	C06730	Benzenoids	苯类
576	Pyrogallol	邻苯三酚	/	87-66-1	C6H6O3	1057	HMDB0013674	C01108	Benzenoids	苯类
577	Phloroglucinol	间苯三酚	/	108-73-6	C6H6O3	359	HMDB0013675	C02183	Benzenoids	苯类
578	3-Hydroxyphenylacetic acid	3-羟基苯乙酸	/	621-37-4	C8H8O3	12122	HMDB0000440	C05593	Benzenoids	苯类
579	2,3-Dihydroxybenzoic acid	2,3-二羟基苯甲酸	/	303-38-8	C7H6O4	19	HMDB0000397	C00196	Benzenoids	苯类
580	4-Hydroxycinnamic acid	4-羟基肉桂酸	/	501-98-4	C9H8O3	637542	HMDB0002035	C00811	Benzenoids	苯类
581	3-(3-Hydroxyphenyl)propanoic acid	3-(3-羟基苯基)丙酸	/	621-54-5	C9H10O3	91	HMDB0000375	C11457	Benzenoids	苯类
582	3,4-Dihydroxyphenylacetic acid	3,4-二羟基苯乙酸	DOPAC	102-32-9	C8H8O4	547	HMDB0001336	C01161	Benzenoids	苯类
583	4-Hydroxyphenylpyruvic acid	4-羟苯丙酮酸	4-HPPA	156-39-8	C9H8O4	979	HMDB0000707	C01179	Benzenoids	苯类
584	3,4-Dihydroxyhydrocinmic acid	3,4-二羟基苯丙酸	/	1078-61-1	C9H10O4	348154	HMDB0000423	C10447	Benzenoids	苯类
585	Catechol	儿茶酚	/	120-80-9	C6H6O2	289	HMDB0000957	C00090	Benzenoids	苯类
586	3,4-Dihydroxybenzaldehyde	3,4-二羟基苯甲醛	/	139-85-5	C7H6O3	8768	HMDB0059965	C16700	Benzenoids	苯类
587	4-Aminobenzoic acid	对氨基苯甲酸	/	150-13-0	C7H7NO2	978	HMDB0001392	C00568	Benzenoids	苯类
588	3-Hydroxyanthranilic acid	3-羟基-2-氨基苯甲酸	3-HAA	548-93-6	C7H7NO3	86	HMDB0001476	C00632	Benzenoids	苯类
589	P-Cresol	对甲苯酚	/	106-44-5	C7H8O	2879	HMDB0001858	C01468	Benzenoids	苯类
590	P-Cresol sulfate	硫酸对甲酚	/	3233-58-7	C7H8O4S	4615423	HMDB0011635	/	Benzenoids	苯类

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591	Phthalic acid	邻苯二甲酸	/	88-99-3	C8H6O4	1017	HMDB0002107	C01606	Benzenoids	苯类
592	Hydroxyphenyllactic acid	羟基苯乳酸	/	306-23-0	C9H10O4	9378	HMDB0000755	C03672	Benzenoids	苯类
593	3-(3,4-Dihydroxyphenyl) Lactic Acid	3-(3,4-二羟基苯基)乳酸	/	23028-17-3	C9H10O5	439435	HMDB0003503	C01207	Benzenoids	苯类
594	Normetanephrine	去甲变肾上腺素	/	97-31-4	C9H13NO3	1237	HMDB0000819	C05589	Benzenoids	苯类
595	Phenylpropiolic acid	苯丙炔酸	/	637-44-5	C9H6O2	69475	HMDB0002359	/	Benzenoids	苯类
596	Acetaminophen	对乙酰氨基酚	/	103-90-2	C8H9NO2	1983	HMDB0001859	C06804	Benzenoids	苯类
597	Benzoylformic acid	苯甲酰甲酸	/	611-73-4	C8H6O3	11915	HMDB0001587	C02137	Benzenoids	苯类
598	3,5-Dihydroxybenzoic acid	3,5-二羟基苯甲酸	/	99-10-5	C7H6O4	7424	HMDB0013677	/	Benzenoids	苯类
599	3-Hydroxybenzoic acid	间羟基苯甲酸	/	99-06-9	C7H6O3	7420	HMDB0002466	C00587	Benzenoids	苯类
600	4-Hydroxybenzaldehyde	4-羟基苯甲醛	/	123-08-0	C7H6O2	126	HMDB0011718	C00633	Benzenoids	苯类
601	Desaminotyrosine	对羟基苯丙酸	/	501-97-3	C9H10O3	10394	HMDB0002199	C01744	Benzenoids	苯类
602	4-Methoxybenzoic Acid	4-甲氧基苯甲酸	/	100-09-4	C8H8O3	7478	HMDB0001101	C02519	Benzenoids	苯类
603	2-Carboxybenzaldehyde	2-羧基苯甲醛	/	119-67-5	C8H6O3	8406	/	C03057	Benzenoids	苯类
604	4-Hydroxy-3-methylbenzoic acid	4-羟基-3-甲基苯甲酸	/	499-76-3	C8H8O3	68138	HMDB0004815	C21167	Benzenoids	苯类
605	2-Hydroxyphenylacetic acid	2-羟基苯乙酸	/	614-75-5	C8H8O3	11970	HMDB0000669	C05852	Benzenoids	苯类
606	2-Methoxyphenyl sulfate	2-甲氧基苯基硫酸	/	3233-59-8	C7H8O5S	22473	HMDB0060013	/	Benzenoids	苯类
607	2-Phenylacetamide	2-苯乙酰胺	/	103-81-1	C8H9NO	7680	HMDB0010715	C02505	Benzenoids	苯类
608	3-Methoxybenzoic acid	3-甲氧基苯甲酸	/	586-38-9	C8H8O3	11461	HMDB0032606	/	Benzenoids	苯类
609	4-Aminophenol	4-氨基苯酚	/	123-30-8	C6H7NO	403	HMDB0001169	C02372	Benzenoids	苯类
610	4-Ethylphenol	4-乙基苯酚	/	123-07-9	C8H10O	31242	HMDB0029306	C13637	Benzenoids	苯类
611	3-Methylcatechol	3-甲基儿茶酚	/	488-17-5	C7H8O2	340	HMDB0301753	C02923	Benzenoids	苯类
612	2-Methylbenzoic acid	2-甲基苯甲酸	/	118-90-1	C8H8O2	8373	HMDB0002340	C07215	Benzenoids	苯类
613	2-Hydroxybenzenepropanoic acid	2-羟基苯丙酸	/	495-78-3	C9H10O3	873	HMDB0033752	C01198	Benzenoids	苯类
614	p-Toluenesulfonic acid	对甲苯磺酸	/	104-15-4	C7H8O3S	6101	HMDB0059933	C06677	Benzenoids	苯类

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615	Phenyl hydrogen sulfate	硫酸苯酯	/	937-34-8	C6H6O4S	74426	HMDB0060015	C02180	Benzenoids	苯类
616	3-Hydroxybenzyl alcohol	3-羟基苯甲醇	/	620-24-6	C7H8O2	102	HMDB0059712	C03351	Benzenoids	苯类
617	3-Hydroxybenzaldehyde	3-羟基苯甲醛	/	100-83-4	C7H6O2	101	/	C03067	Benzenoids	苯类
618	3,4-Dimethoxybenzoic Acid	3,4-二甲氧基苯甲酸	/	93-07-2	C9H10O4	7121	HMDB0059763	/	Benzenoids	苯类
619	4-Methoxyphenylacetic acid	对甲氧基苯乙酸	/	104-01-8	C9H10O3	7690	HMDB0002072	/	Benzenoids	苯类
620	3,4,5-Trimethoxybenzoic Acid	3,4,5-三甲氧基苯甲酸	/	118-41-2	C10H12O5	8357	HMDB0033839	/	Benzenoids	苯类
621	2,6-Dihydroxybenzoic acid	2,6-二羟基苯甲酸	/	303-07-1	C7H6O4	9338	HMDB0013676	C21298	Benzenoids	苯类
622	3-(3,4-Dimethoxyphenyl) Propionic Acid	3-(3,4-二甲氧基苯基)丙酸	/	2107-70-2	C11H14O4	75019	/	/	Benzenoids	苯类
623	2-Aminophenol	2-氨基苯酚	/	95-55-6	C6H7NO	5801	/	C01987	Benzenoids	苯类
624	O-Succinylbenzoate	O-琥珀酰苯甲酸	/	27415-09-4	C11H10O5	955	HMDB0304087	C02730	Benzenoids	苯类
625	Quinolinic acid	喹啉酸	QA	89-00-9	C7H5NO4	1066	HMDB0000232	C03722	Pyridines	吡啶类
626	4-Pyridoxic acid	4-吡哆酸	/	82-82-6	C8H9NO4	6723	HMDB0000017	C00847	Pyridines	吡啶类
627	2-Hydroxypyridine	2-羟基吡啶	/	72762-00-6	C5H5NO	8871	HMDB0013751	C02502	Pyridines	吡啶类
628	6-Hydroxynicotinic acid	6-羟基烟酸	/	5006-66-6	C6H5NO3	72924	HMDB0002658	C01020	Pyridines	吡啶类
629	Isonicotinic acid	异烟酸	/	55-22-1	C6H5NO2	5922	HMDB0060665	C07446	Pyridines	吡啶类
630	Trigonelline	葫芦巴碱	/	535-83-1	C7H7NO2	5570	HMDB0000875	C01004	Pyridines	吡啶类
631	N-Methylnicotinamide	N-甲基烟酰胺	/	114-33-0	C7H8N2O	64950	HMDB0003152	/	Pyridines	吡啶类
632	Nicotine	烟碱	/	54-11-5	C10H14N2	89594	HMDB0001934	C00745	Pyridines	吡啶类
633	4,6-Dihydroxyquinoline	4,6-二羟基喹啉	/	3517-61-1	C9H7NO2	440738	HMDB0004077	C05639	Pyridines	吡啶类
634	Nicotinamide adenine dinucleotide phosphate	氧化型辅酶II	NADP	53-59-8	C21H28N7O17P3	5885	HMDB0000217	C00006	Others	其他
635	Coenzyme A	辅酶 A	CoA	85-61-0	C21H36N7O16P3S	87642	HMDB0001423	C00010	Others	其他
636	Dephospho-CoA	脱磷辅酶 A	/	3633-59-8	C21H35N7O13P2S	444485	HMDB0001373	C00882	Others	其他
637	9S-hydroxy-10E,12Z-octadecadienoic acid	9S-羟基-10E,12Z-十八碳二烯酸	9S-HODE	73543-67-6	C18H32O3	5312830	HMDB0062652	C14767	Others	其他

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638	(±)19,20-dihydroxy-4Z,7Z,10Z,13Z,16Z-docosapentaenoic acid	(±)19,20-二羟基-4Z,7Z,10Z,13Z,16Z-二十二碳五烯酸	±19,20-DiHDPA	/	C22H34O4	16061148	HMDB0010214	/	Others	其他
639	Glycerophosphocholine	甘油磷酰胆碱	/	28319-77-9	C8H20NO6P	657272	HMDB0000086	C00670	Others	其他
640	Maltol	麦芽酚	/	118-71-8	C6H6O3	8369	HMDB0030776	C11918	Others	其他
641	Biotin	生物素	/	58-85-5	C10H16N2O3S	171548	HMDB0000030	C00120	Others	其他
642	Allantoin	尿囊素	/	97-59-6	C4H6N4O3	204	HMDB0000462	C01551	Others	其他
643	Urocanic acid	尿刊酸	/	104-98-3	C6H6N2O2	736715	HMDB0000301	C00785	Others	其他
644	Imidazole	咪唑	/	288-32-4	C3H4N2	795	HMDB0001525	C01589	Others	其他
645	Methylguanidine	甲基胍	/	471-29-4	C2H7N3	10111	HMDB0001522	C02294	Others	其他
646	Ciliatine	氨乙基膦酸	/	2041-14-7	C2H8NO3P	339	HMDB0011747	C03557	Others	其他
647	Imidazoleacetic acid	咪唑乙酸	/	645-65-8	C5H6N2O2	96215	HMDB0002024	C02835	Others	其他
648	4-Guanidinobutyric acid	4-胍基丁酸	/	463-00-3	C5H11N3O2	500	HMDB0003464	C01035	Others	其他
649	2',4'-Dihydroxyacetophenone	2',4'-二羟基苯乙酮	/	89-84-9	C8H8O3	6990	HMDB0029659	C03663	Others	其他
650	Lipoamide	硫辛酰胺	LM	940-69-2	C8H15NOS2	863	HMDB0000962	C00248	Others	其他
651	Phosphocreatine	肌酐磷酸	/	67-07--2	C4H10N3O5P	587	HMDB0001511	C02305	Others	其他
652	3-Pyridol	3-羟基吡啶	/	109-00-2	C5H5NO	7971	/	/	Others	其他
653	Dimethylbenzimidazole	5,6-二甲基苯并咪唑	/	582-60-5	C9H10N2	675	HMDB0003701	C03114	Others	其他
654	Urea	尿素	/	57-13-6	CH4N2O	1176	HMDB0000294	C00086	Others	其他
655	Mevalonolactone	甲羟戊酸内酯	/	674-26-0	C6H10O3	10428	HMDB0244840	/	Others	其他
656	Pyrrolidine	吡咯烷	/	123-75-1	C4H9N	31268	HMDB0031641	/	Others	其他
657	2-Oxindole	2-吲哚酮	/	59-48-3	C8H7NO	321710	HMDB0061918	C12312	Others	其他
658	Quinoline-2-carboxylic acid	喹啉-2-甲酸	/	93-10-7	C10H7NO2	7124	HMDB0000842	C06325	Others	其他
659	5-Hydroxymethyl-2-furancarboxylic acid	5-羟甲基-2-呋喃甲酸	/	6338-41-6	C6H6O4	80642	HMDB0002432	C20448	Others	其他
660	4-Aminoimidazole	4-氨基咪唑	/	4919-03-3	C3H5N3	484	HMDB0003929	C05239	Others	其他

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661	1-Methyl-Hydantoin	1-甲基乙内酰脲	/	616-04-6	C4H6N2O2	69217	HMDB0003646	C02565	Others	其他
662	4-Hydroxycinnamoylagmatine	4-羟基肉桂酰精胺	/	7295-86-5	C14H20N4O2	5280691	HMDB0033460	C04498	Others	其他
663	Urobilin	尿胆素	/	1856-98-0	C33H42N4O6	6433298	/	/	Others	其他
664	Phenylethanolamine	苯乙醇胺	/	7568-93-6	C8H11NO	1000	HMDB0001065	C02735	Others	其他
665	2,3-Heptanedione	2,3-庚二酮	/	96-04-8	C7H12O2	60983	HMDB0031476	/	Others	其他
666	2,8-Quinolinediol	2,8-二羟基喹啉	/	15450-76-7	C9H7NO2	97250	HMDB0240311	C06342	Others	其他
667	Ethyl Sulfate	硫酸乙酯	/	540-82-9	C2H6O4S	6004	HMDB0031233	/	Others	其他
668	N,N-Dimethylphenylethylamine	N,N-二甲基苯乙胺	/	1126-71-2	C10H15N	25125	/	/	Others	其他
669	Malonaldehyde	丙二醛	/	542-78-9	C3H4O2	10964	HMDB0006112	C19440	Others	其他

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