

# Supplementary supporting Data

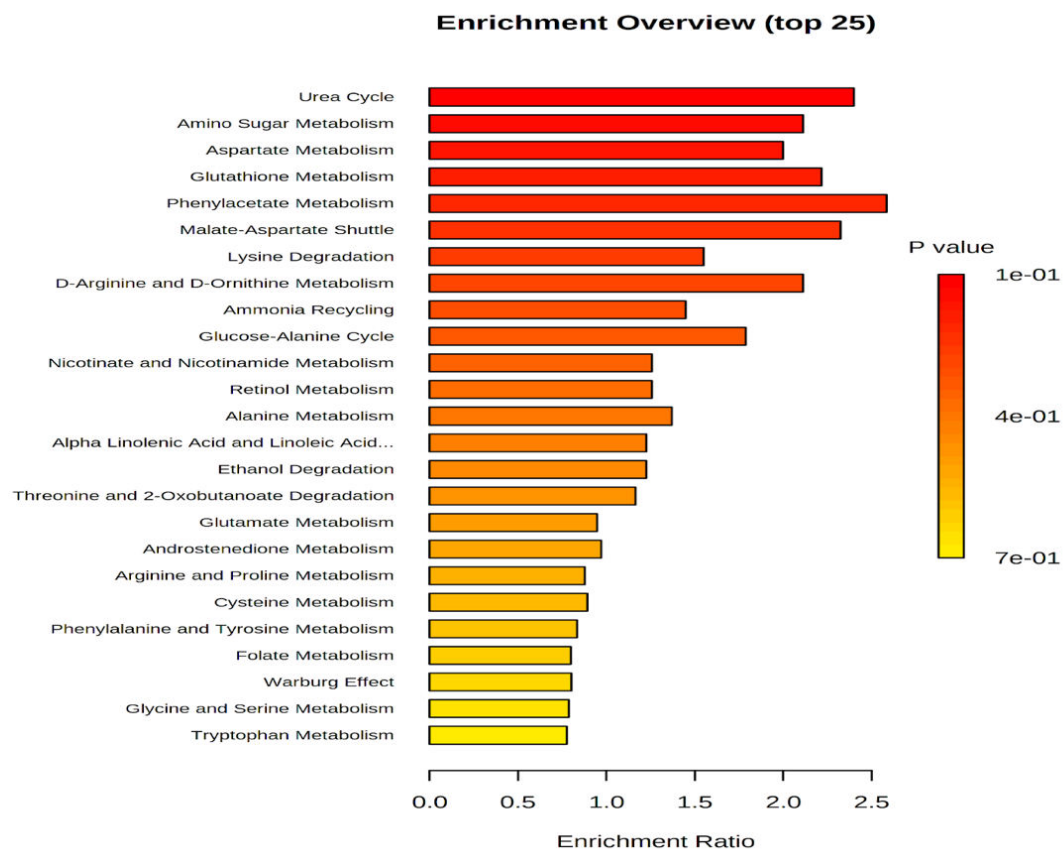
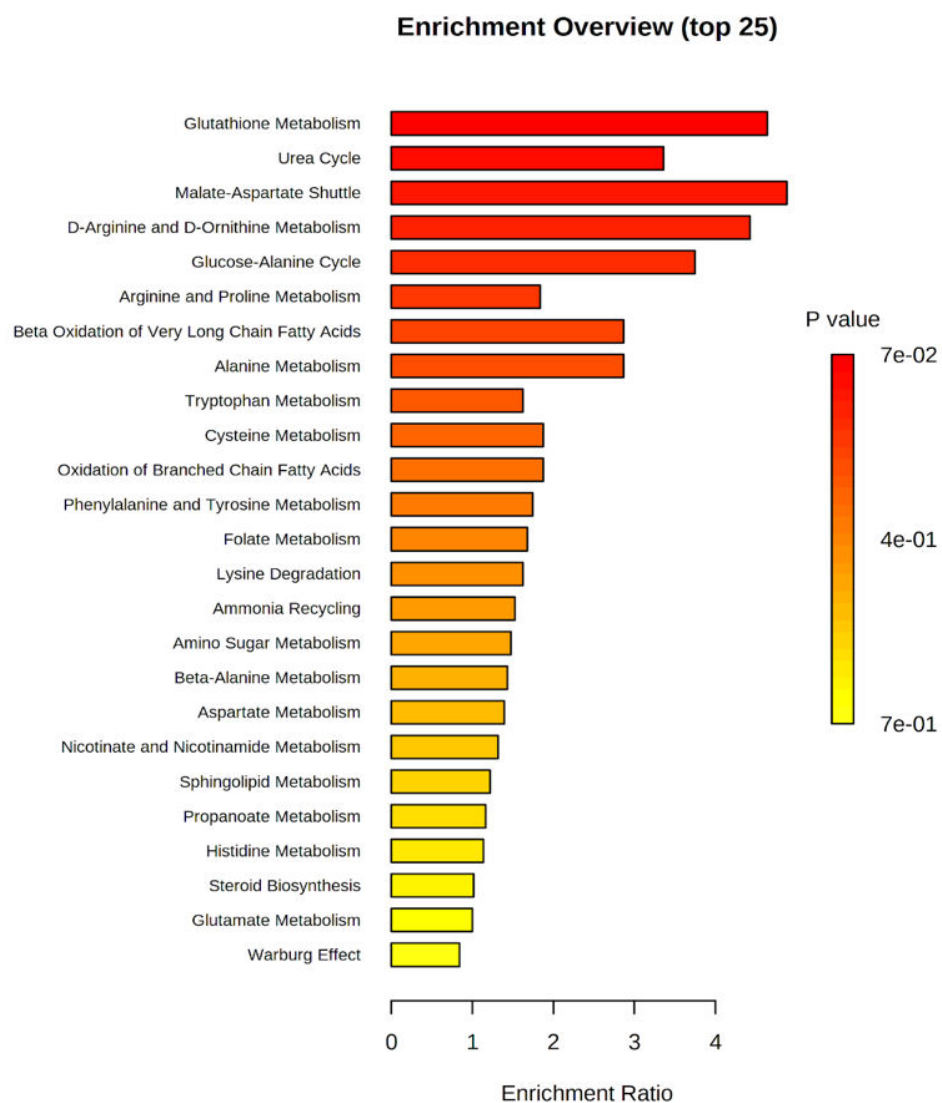
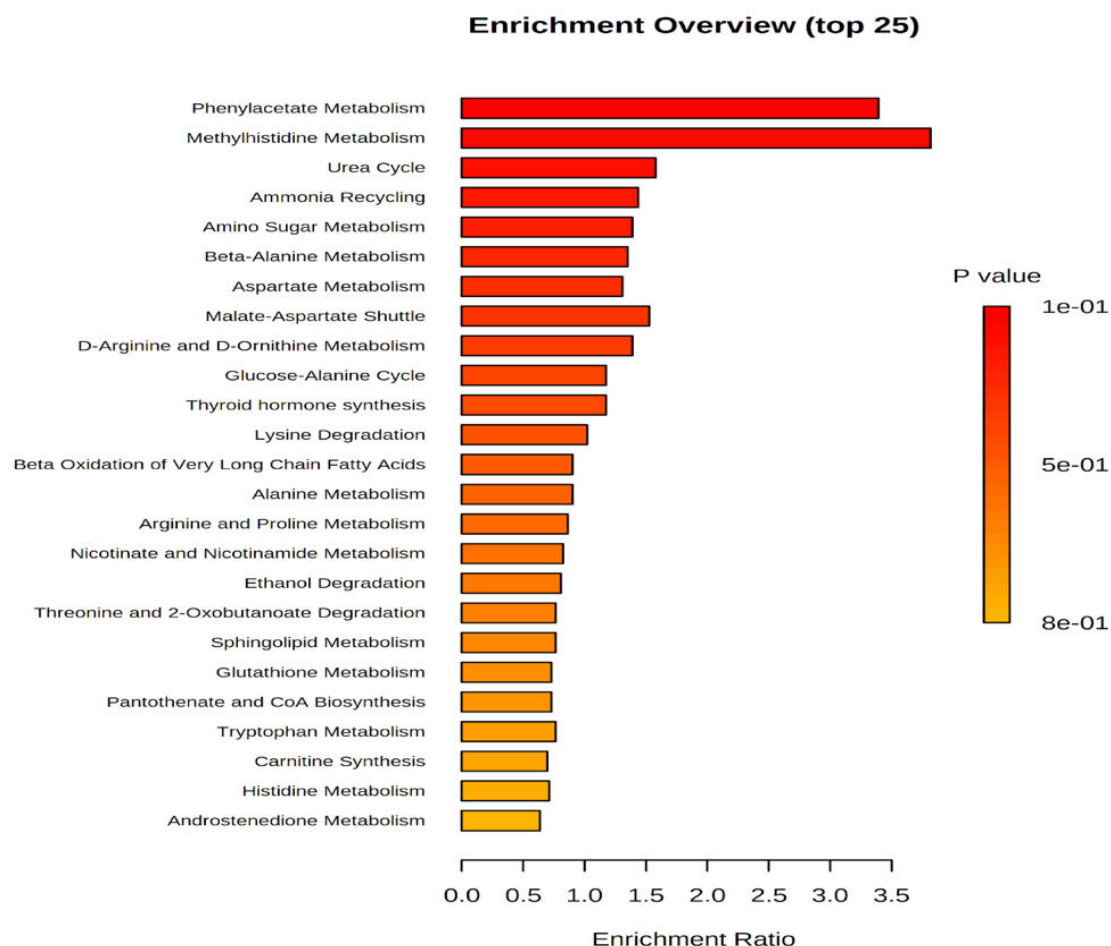


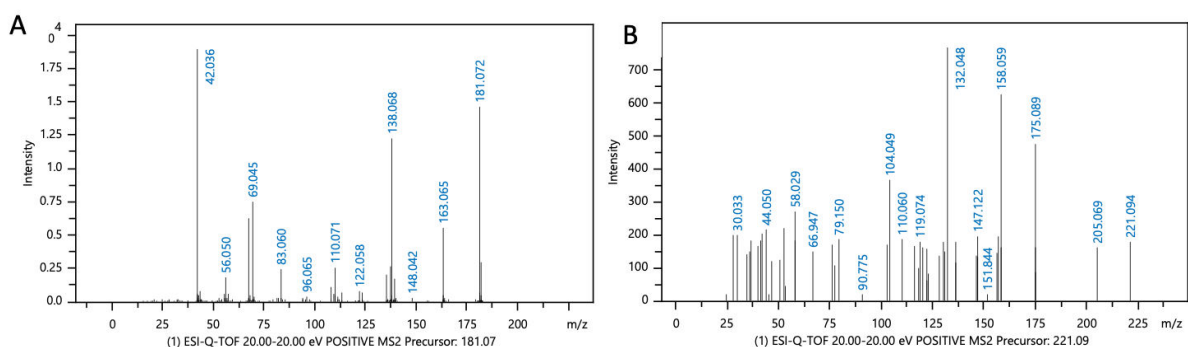
Figure S1: (A) Enrichment Analysis of Controls and Normoglycemic MetS



**Figure S1: (B) Enrichment Analysis of Normoglycemic MetS and Prediabetic MetS**



**Figure S1: (C) Enrichment Analysis of Controls and Prediabetic MetS**



**Figure S2: Mass spectra for L-sorbose (A) and 5-Hydroxy-L-tryptophan (B)**

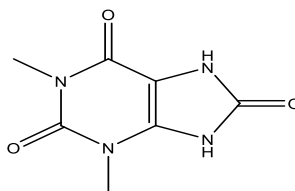
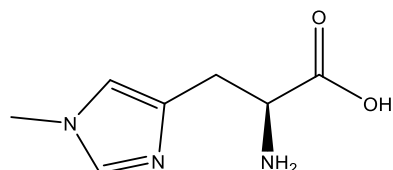
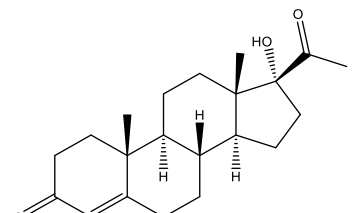
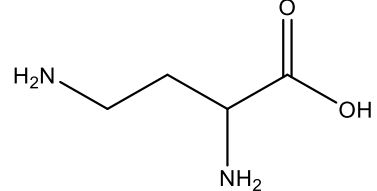
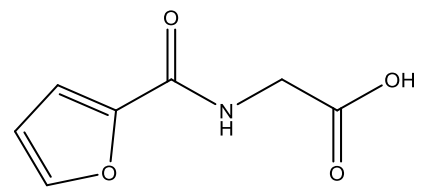
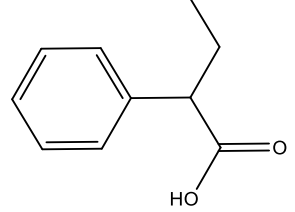
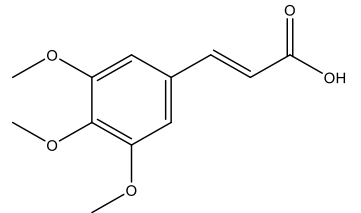
**Table S1:** Retention time and MS/MS

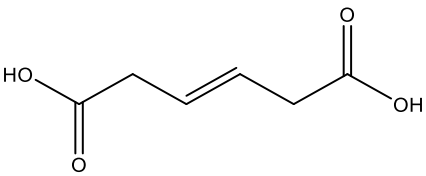
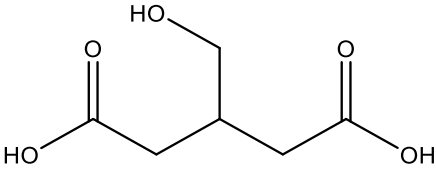
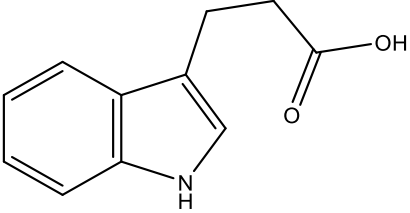
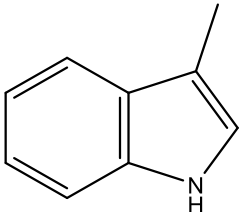
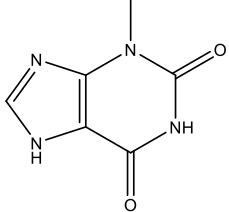
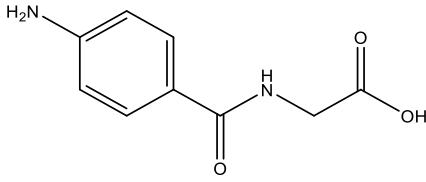
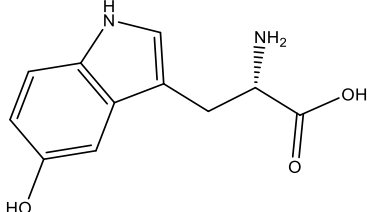
Name	RT [min]	m/z measured	Mass measured
1,3-Dimethyluric acid	9.75	197.06728	196.06
1-Methylhistidine	1.85	170.09301	169.08574
17-Hydroxyprogesterone	22.39	331.22326	330.21598
2,4-Diaminobutyric acid	17.41	119.08565	118.07837
2-Furoylglycine	3.34	170.04212	169.03485
2-Phenylbutyric acid	13.42	147.08064	164.08397
3,4,5-Trimethoxycinnamic acid	10.68	239.09168	238.08441
3-Hexenedioic acid	3.59	145.04942	144.04214
3-Hydroxymethylglutaric acid	3.53	163.06006	162.05278
3-Indolepropionic acid	12.32	190.08703	189.07976
3-Methylindole	9.3	132.08086	131.07359
3-Methylxanthine	8.85	167.05661	166.04934
4-Aminohippuric acid	8.72	195.07649	194.06921
5-Hydroxy-L-tryptophan	9.54	221.09233	220.08505
5-Hydroxyindoleacetic acid	8.86	192.06586	191.05859
5-Hydroxylysine	13.29	163.1118	162.10453
9-Methyluric acid	8.85	183.05181	182.04454
Acetic acid	11.5	61.0283	60.02102
All-trans-retinoic acid	15.24	301.21685	300.20957
Allantoic acid	1.9	177.06127	176.054
Alpha-Tocopherol	20.31	431.38435	430.37708
Androstenedione	15.01	287.2006	286.19332
Androsterone	17.81	291.23018	290.2229
Benzamide	8.98	122.05785	121.05057
Benzoic acid	5.9	123.04392	122.03664
Biotin	9.31	245.09839	244.09111
Caffeine	9.79	195.08803	194.08075
Cinnamic acid	8.85	149.06018	148.0529
Creatine	2.39	132.07678	131.0695
Creatinine	2.37	114.06616	113.05888
D-Alanine	2.39	90.05527	89.04799
Deoxycholic acid glycine conjugate	14.1	450.32217	449.31425
DL-2-aminooctanoic acid	2.45	160.13322	159.12595
Elaidic acid	0.71	283.26283	282.25555
Estradiol	13.24	273.18528	272.178
Gamma-terpinene	16.95	137.13267	136.12539

Glycerophosphocholine	2.19	280.09216	257.10294
Glycine	3.47	76.03958	75.0323
Glycyl-L-leucine	9.25	189.12393	188.11666
Guanidine	2.66	60.05568	59.04841
Heptadecanoic acid	26.01	271.2634	270.25612
Hippuric acid	10.57	202.04784	179.05857
Homoveratric acid	10.93	197.07839	196.07112
Hyodeoxycholic acid	21.52	393.29695	392.28968
Indole	9.18	118.06528	117.05801
Indole-3-carbinol	9.44	148.07568	147.0684
Indoleacetic acid	11.62	176.0709	175.06363
Indolelactic acid	11.61	206.08113	205.07385
Isovalerylcarnitine	9.44	246.17081	245.16353
L-Acetylcarnitine	3.94	204.12305	203.11578
L-Arginine	2.67	175.11914	174.11186
L-Aspartyl-L-phenylalanine	9.91	281.1136	280.10633
L-Carnitine	2.63	162.11239	161.10511
L-Glutamic acid	3.52	148.06045	147.05317
L-Glutamine	10.02	147.07664	146.06937
L-Histidine	1.82	156.07692	155.06964
L-Kynurenine	9.4	209.09204	208.08477
L-Lysine	2.7	147.11326	146.10598
L-Methionine	3.84	150.05858	149.0513
L-Norleucine	4.76	132.10191	131.09463
L-Proline	2.67	116.0706	115.06333
L-Sorbose	9.67	181.07229	180.06501
L-Threonine	9.73	120.06559	119.05832
L-Tryptophan	9.82	205.09712	204.08984
L-Valine	2.68	118.08619	117.07892
Linoleic acid	17.79	281.24755	280.24027
m-Aminobenzoic acid	2.39	160.03472	137.04564
m-Coumaric acid	5.82	165.05461	164.04734
Medroxyprogesterone	16.47	345.24287	344.23559
N,N-Dimethylformamide	2.66	74.06024	73.05296
Nonadecanoic acid	29.91	299.29499	298.28772
Normetanephine	2.33	184.09468	183.0874
Nutriacholic acid	21.43	413.26578	390.27682
o-Tyrosine	3.81	182.0814	181.07413
p-Octopamine	4.14	154.08392	153.07665

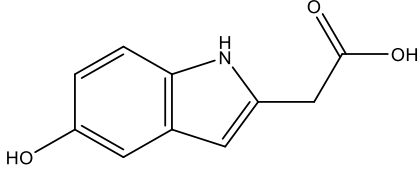
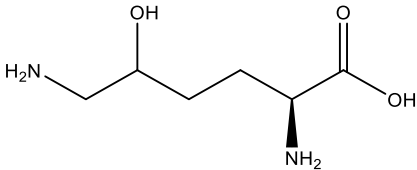
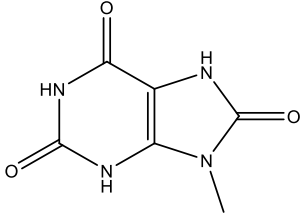
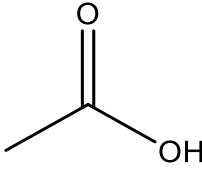
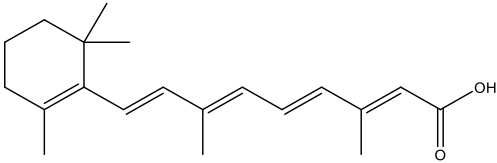
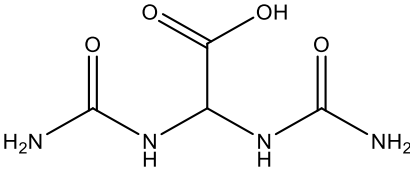
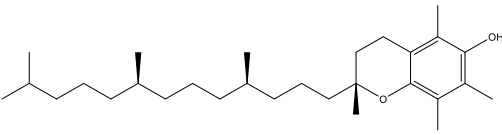
Paraxanthine	9.88	181.07204	180.06476
PC(16:0/16:0)	20.32	734.56788	733.5606
Phenylacetaldehyde	14.42	121.06472	120.05745
Phenylacetic acid	12.9	137.05962	136.05235
Pipecolic acid	1.79	130.08625	129.07898
Pregnenolone	19.15	317.24822	316.24094
Pregnenolone sulfate	15.32	397.20054	396.19326
Pyridoxamine	9.54	169.09724	168.08997
Pyroglutamic acid	3.76	130.04995	129.04267
Quinaldic acid	8.87	174.05556	173.04828
Retinal	17.58	285.22164	284.21436
Saccharopine	16.52	277.13545	276.12817
Sphinganine	13.15	302.30576	301.29849
Sphingosine	13.51	282.27948	299.28278
Stearic acid	24.6	285.27764	284.27037
Threonic acid	4.87	137.04577	136.03849
Thymol	17.45	151.11199	150.10471
Thyroxine	12.35	777.69442	776.68715
Traumatic acid	10.83	229.14156	228.13429
Trimethylamine	20.45	60.08098	59.0737
Urea	22.82	61.03982	60.03254
Uric acid	4.94	169.03565	168.02837
Uridine	14.87	245.07889	244.07161
Vitamin D3	22.01	385.34666	384.33938

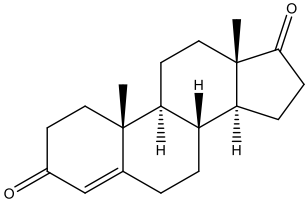
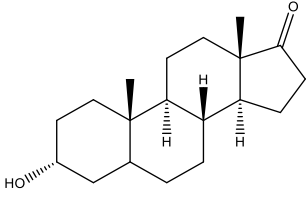
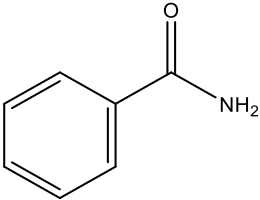
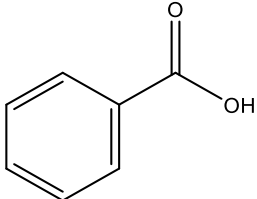
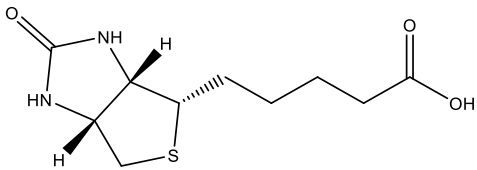
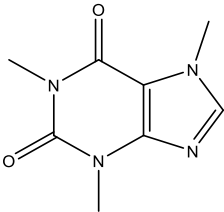
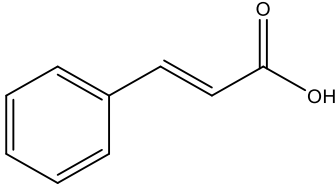
**Table S2: Chemical structures of metabolites**

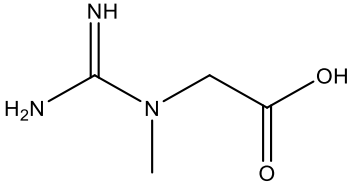
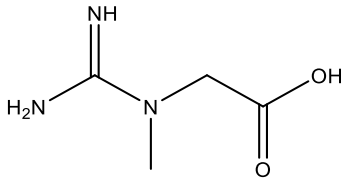
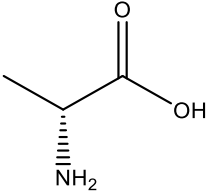
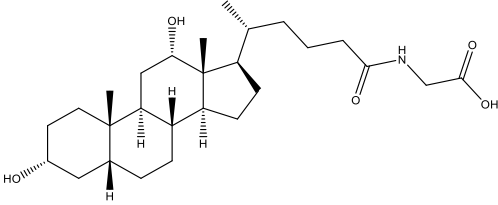
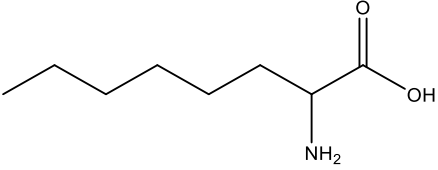
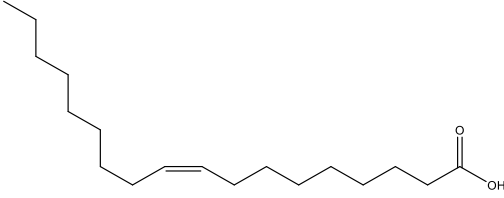
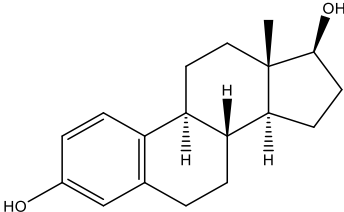
Name	Chemical Structure
1,3-Dimethyluric acid	
1-Methylhistidine	
17-Hydroxyprogesterone	
2,4-Diaminobutyric acid	
2-Furoylglycine	
2-Phenylbutyric acid	
3,4,5-Trimethoxycinnamic acid	

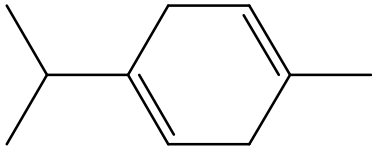
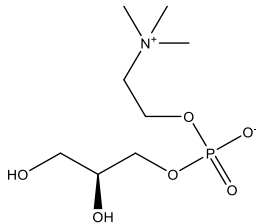
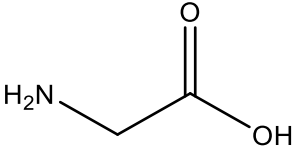
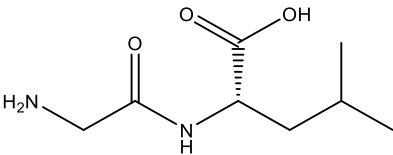
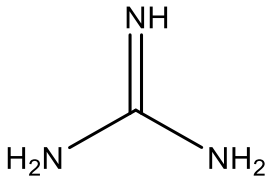
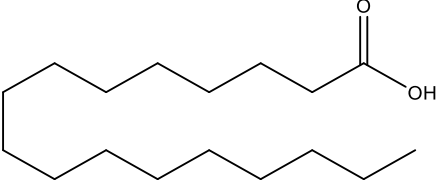
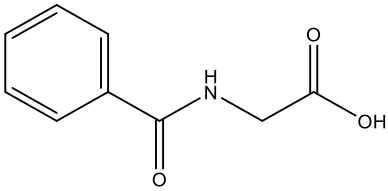
<b>3-Hexenedioic acid</b>	
<b>3-Hydroxymethylglutaric acid</b>	
<b>3-Indolepropionic acid</b>	
<b>3-Methylindole</b>	
<b>3-Methylxanthine</b>	
<b>4-Aminohippuric acid</b>	
<b>5-Hydroxy-L-tryptophan</b>	

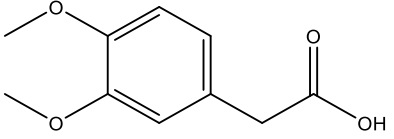
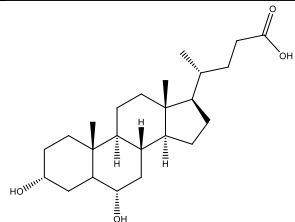
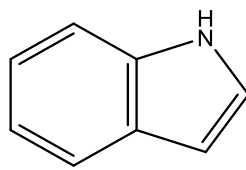
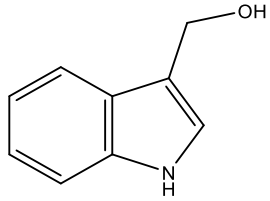
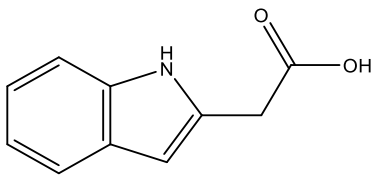
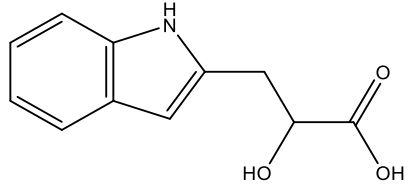
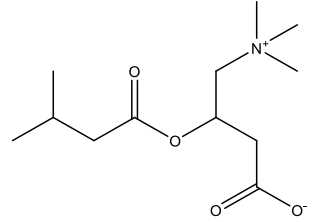


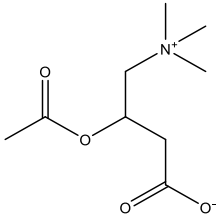
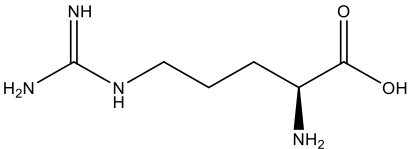
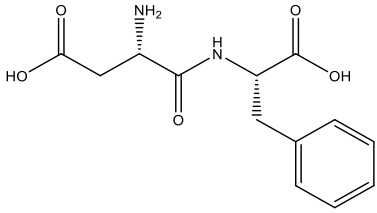
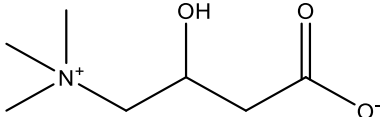
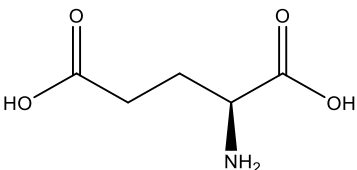
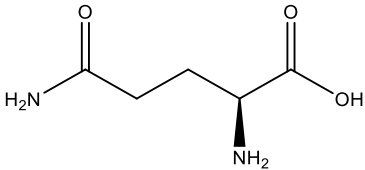
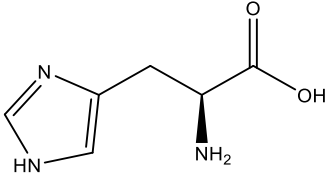
<b>5-Hydroxyindoleacetic acid</b>	
<b>5-Hydroxylysine</b>	
<b>9-Methyluric acid</b>	
<b>Acetic acid</b>	
<b>All-trans-retinoic acid</b>	
<b>Allantoic acid</b>	
<b>Alpha-Tocopherol</b>	

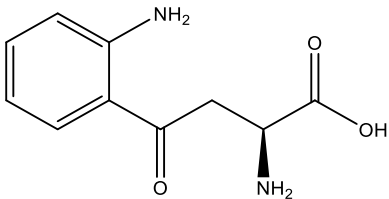
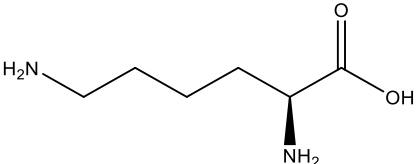
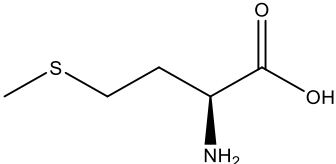
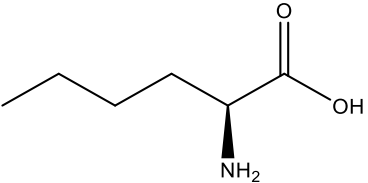
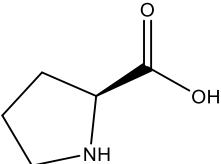
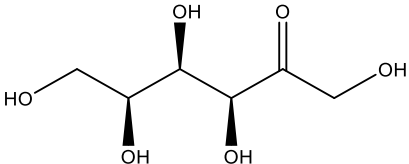
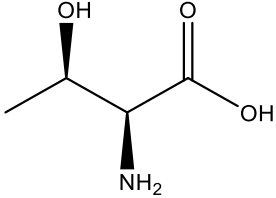
<b>Androstenedione</b>	
<b>Androsterone</b>	
<b>Benzamide</b>	
<b>Benzoic acid</b>	
<b>Biotin</b>	
<b>Caffeine</b>	
<b>Cinnamic acid</b>	

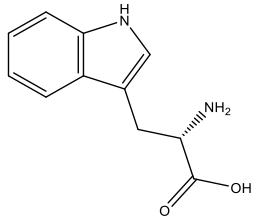
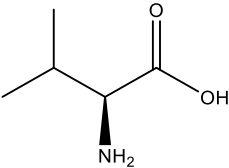
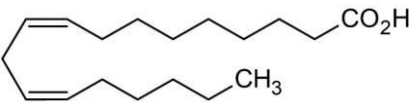
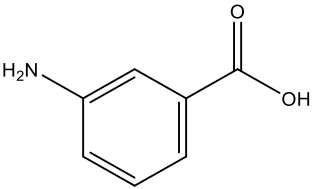
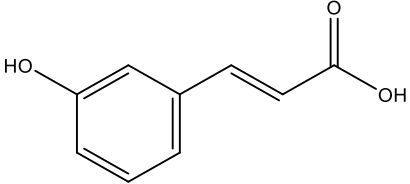
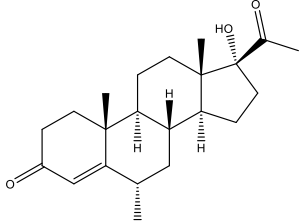
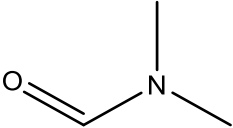
<b>Creatine</b>	
<b>Creatinine</b>	
<b>D-Alanine</b>	
<b>Deoxycholic acid glycine conjugate</b>	
<b>DL-2-aminooctanoic acid</b>	
<b>Elaidic acid</b>	
<b>Estradiol</b>	

<b>Gamma-terpinene</b>	
<b>Glycerophosphocholine</b>	
<b>Glycine</b>	
<b>Glycyl-L-leucine</b>	
<b>Guanidine</b>	
<b>Heptadecanoic acid</b>	
<b>Hippuric acid</b>	

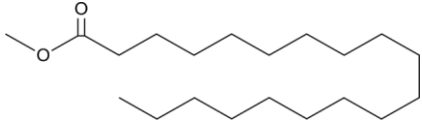
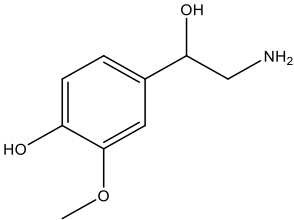
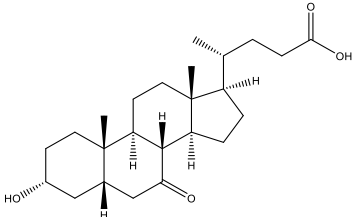
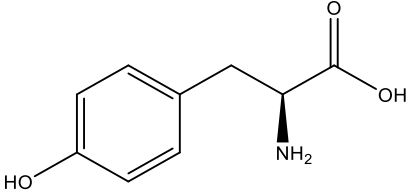
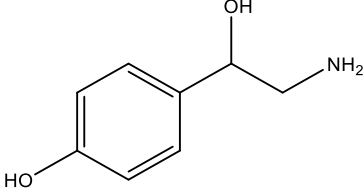
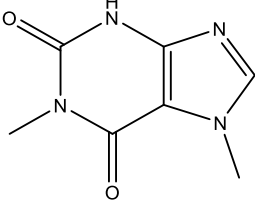
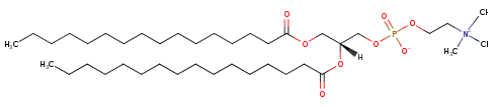
<b>Homoveratric acid</b>	
<b>Hyodeoxycholic acid</b>	
<b>Indole</b>	
<b>Indole-3-carbinol</b>	
<b>Indoleacetic acid</b>	
<b>Indolelactic acid</b>	
<b>Isovalerylcarnitine</b>	

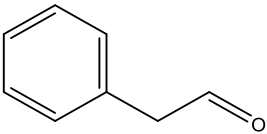
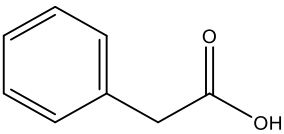
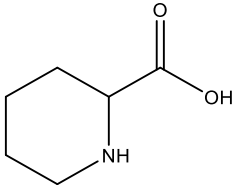
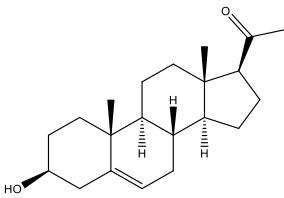
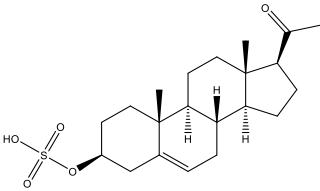
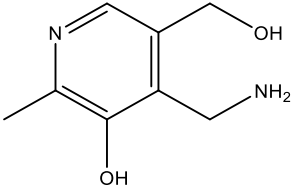
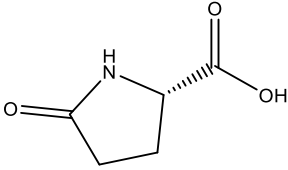
<b>L-Acetylcarnitine</b>	
<b>L-Arginine</b>	
<b>L-Aspartyl-L-phenylalanine</b>	
<b>L-Carnitine</b>	
<b>L-Glutamic acid</b>	
<b>L-Glutamine</b>	
<b>L-Histidine</b>	

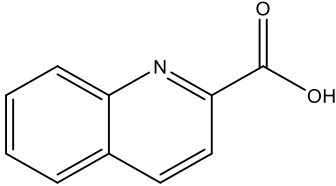
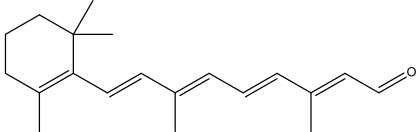
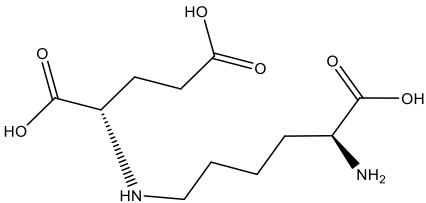
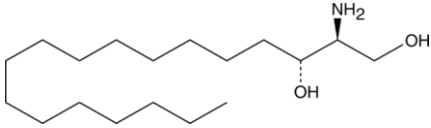
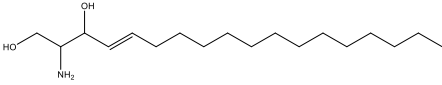
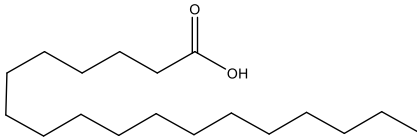
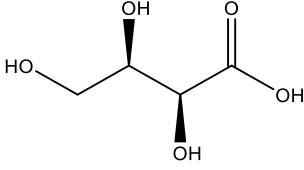
<b>L-Kynurenine</b>	
<b>L-Lysine</b>	
<b>L-Methionine</b>	
<b>L-Norleucine</b>	
<b>L-Proline</b>	
<b>L-Sorbose</b>	
<b>L-Threonine</b>	

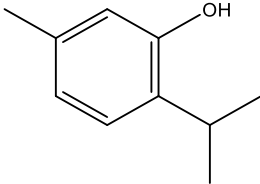
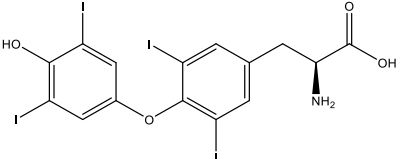
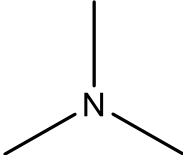
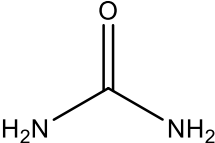
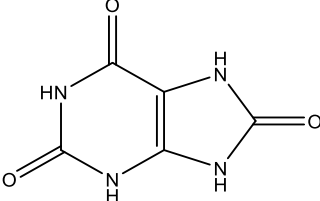
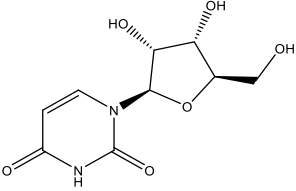
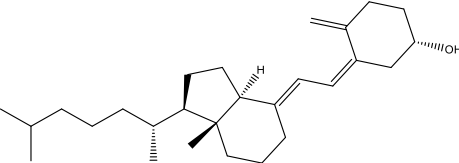
<b>L-Tryptophan</b>	
<b>L-Valine</b>	
<b>Linoleic acid</b>	
<b>m-Aminobenzoic acid</b>	
<b>m-Coumaric acid</b>	
<b>Medroxyprogesterone</b>	
<b>N,N-Dimethylformamide</b>	

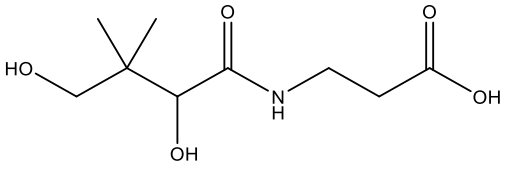
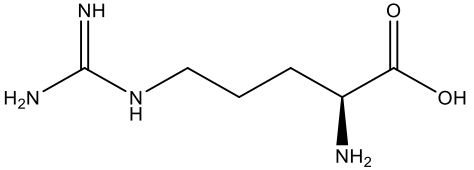
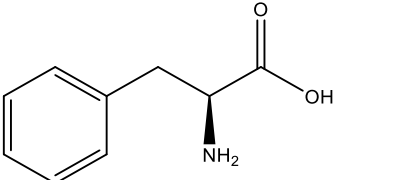
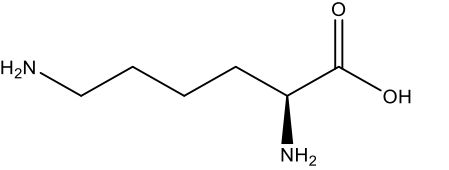
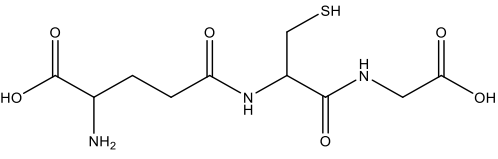


<b>Nonadecanoic acid</b>	
<b>Normetanephrine</b>	
<b>Nutriacholic acid</b>	
<b>o-Tyrosine</b>	
<b>p-Octopamine</b>	
<b>Paraxanthine</b>	
<b>PC(16:0/16:0)</b>	

<b>Phenylacetaldehyde</b>	
<b>Phenylacetic acid</b>	
<b>Pipecolic acid</b>	
<b>Pregnenolone</b>	
<b>Pregnenolone sulfate</b>	
<b>Pyridoxamine</b>	
<b>Pyroglutamic acid</b>	

<b>Quinaldic acid</b>	
<b>Retinal</b>	
<b>Saccharopine</b>	
<b>Sphinganine</b>	
<b>Sphingosine</b>	
<b>Stearic acid</b>	
<b>Threonic acid</b>	

<b>Thymol</b>	
<b>Thyroxine</b>	
<b>Trimethylamine</b>	
<b>Urea</b>	
<b>Uric acid</b>	
<b>Uridine</b>	
<b>Vitamin D3</b>	

<b>Pantothenic acid</b>	
<b>Arginine</b>	
<b>Phenylalanine</b>	
<b>Lysine</b>	
<b>Glutathione</b>	
<b>Glyoxylate Dicarboxylate Conjugate</b>	