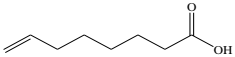
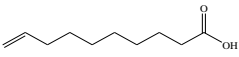
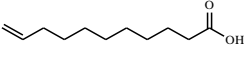
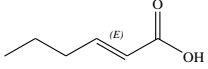
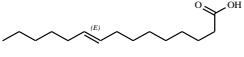
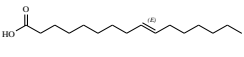
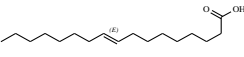
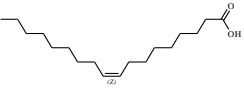
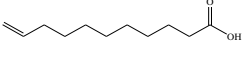


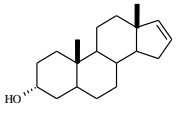
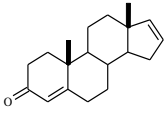
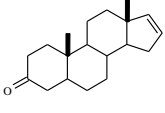
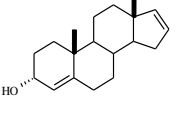
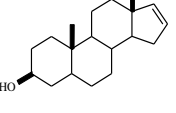
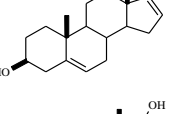
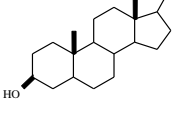
## Appendix A

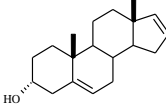
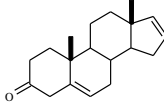
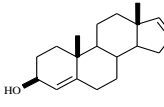
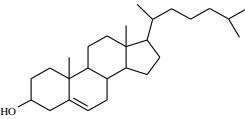
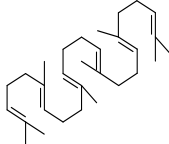
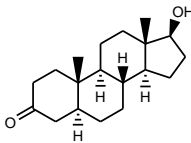
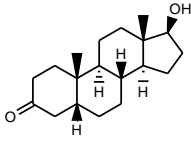
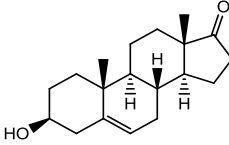
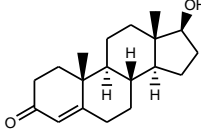
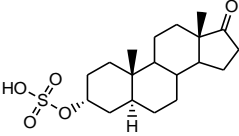
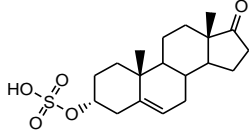
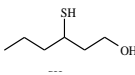
A list of reported metabolites found in human apocrine sweat secretions. For further information see Appendix A on the attached CD

Components	Structure	Molecule	Mass	M+H
<b>3-Hydroxy acids</b>				
3-Hydroxy-3-methylhexanoic acid		C7H14O3	146.0943	147.1021
3-Hydroxy-4-methylhexanoic acid		C7H14O3	146.0943	147.1021
3-Hydroxy-3-methylheptanoic acid		C8H16O3	160.1099	161.0628
3-Hydroxy-4-methylheptanoic acid		C8H16O3	160.1099	161.0628
3-Hydroxyoctanoic acid		C8H16O3	160.1099	161.0628
3-Hydroxy-3-methyloctanoic acid		C9H18O3	174.1256	175.1334
3-Hydroxy-4-methyloctanoic acid		C9H18O3	174.1256	175.1334
3-Hydroxy-4-methylnonanoic acid		C10H20O3	188.1412	189.1491
3-Hydroxydecanoic acid		C10H20O3	188.1412	189.1491
<b>Unsaturated acids</b>				
(Z)-3-Methylhex-2-enoic acid		C7H12O2	128.0837	129.0916
(E)-3-Methylhex-2-enoic acid		C7H12O2	128.0837	129.0916
4-Methyloct-4-enoic acid		C9H16O2	156.1150	157.1229
(Z)-4-Methyloct-3-enoic acid		C9H16O2	156.1150	157.1229
(E)-4-Methyloct-3-enoic acid		C9H16O2	156.1150	157.1229
(Z)-4-Methylnon-3-enoic acid		C10H18O2	170.1307	171.1385
(E)-4-Methylnon-3-enoic acid		C10H18O2	170.1307	171.1385
(E)-3-Methyl-2-octenoic acid		C9H16O2	156.1150	157.1229
(E)-3-Methyl-2-pentenoic acid		C6H10O2	114.0681	115.0759
(Z)-3-Methylhex-2-enoic acid		C7H12O2	128.0837	129.0916

7-Octenoic acid		C8H14O2	142.0994	143.1072
9-Decenoic acid		C10H18O2	170.1307	171.1385
10-Undecenoic acid		C11H20O2	184.1463	185.1542
2-Hexenoic acid		C6H10O2	114.0681	115.0759
9-Pentadecenoic acid		C15H28O2	240.2089	241.2168
9-Hexadecenoic acid		C16H30O2	254.2246	255.2324
9-Heptadecenoic acid		C17H32O2	268.2402	269.2481
Oleic acid		C18H34O2	282.2559	283.2637
Unsaturated C11 acid (10-undecenoic acid)		C11H20O2	184.1463	185.1542

### Steroidal

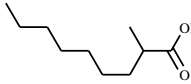
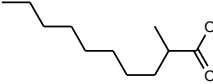
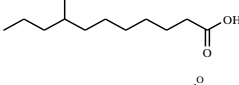
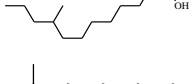
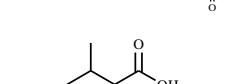
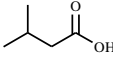
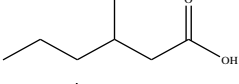
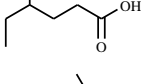
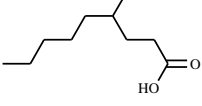
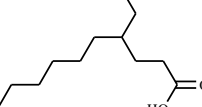

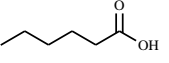
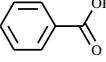
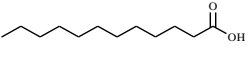
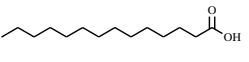
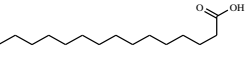
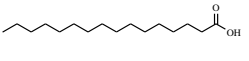
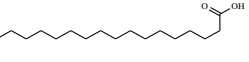
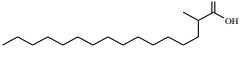
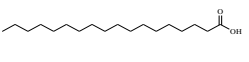
5 $\alpha$ -Androst-16-en-3 $\alpha$ -ol		C19H30O	274.2297	275.2375
Androsta-4, 16-dien-3-one		C19H26O	270.1984	271.2062
5 $\alpha$ -Androst-16-en-3-one		C19H28O	272.2140	273.2218
Androsta-4, 16-dien-3 $\alpha$ -ol		C19H28O	272.2140	273.2218
5 $\alpha$ -Androst-16-en-3 $\beta$ -ol		C19H30O	274.2297	275.2375
5 $\alpha$ -Androsta-5, 16-dien-3 $\beta$ -ol		C19H28O	272.2140	273.2218
Androst-5-ene-3 $\beta$ -17 $\alpha$ / $\beta$ -diols		C19H32O2	292.2402	293.2481

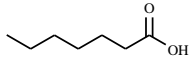
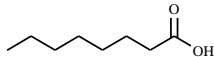
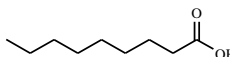
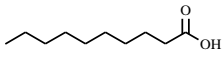
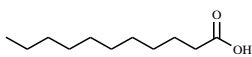
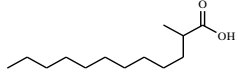
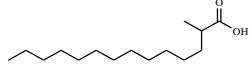
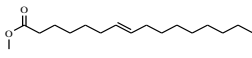
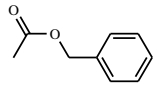
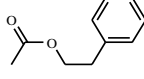
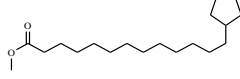
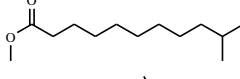
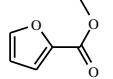
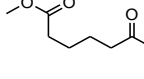
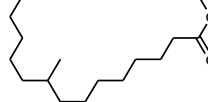
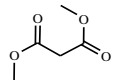
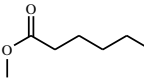
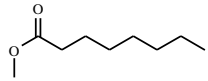
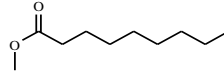
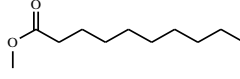
Androsta-5, 16-dien-3 $\alpha$ -ol		C19H28O	272.2140	273.2218	
Androsta-5, 16-dien-3-one		C19H26O	270.1984	271.2062	
Androsta-4, 16-dien-3 $\alpha$ -ol		C19H28O	272.2140	273.2218	
Cholesterol		C27H46O	386.3549	387.3627	
Squalene		C30H50	410.3913	411.3991	
5 $\alpha$ -Dihydrotestosterone		C19H30O2	290.2246	291.2324	
5 $\beta$ -Dihydrotestosterone		C19H30O2	290.2246	291.2324	
Dehydrocpiandrosterone		C19H28O2	288.2089		
Testosterone		C19H28O2	288.2089	289.2168	
17-Oxo-5 $\alpha$ -androstan-3 $\alpha$ -yl sulfate		C19H30O5S	370.1814	371.1892	
17-Oxo-5 $\alpha$ -androsten-3 $\alpha$ -yl sulfate		C19H28O5S	368.1657	369.1736	
<b>Sulfanylalkanols</b>					
3-Sulfanylhexasan-1-ol		C6H14OS	134.0765	135.0844	

2-Methyl-3-sulfanylbutan-1-ol		C5H12OS	120.0609	121.0687
3-Sulfanylpentan-1-ol		C5H12OS	120.0609	121.0687
3-Methyl-3-sulfanylohexan-1-ol		C7H16OS	148.0922	149.1000
Dimethylsulfone		C2H6O2S	94.0089	95.0167

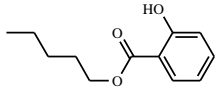
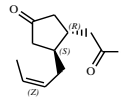
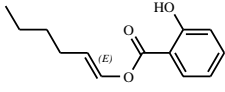
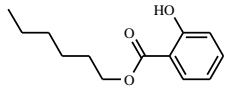
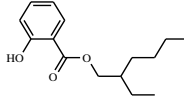
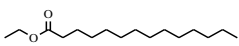
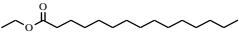
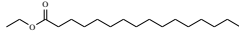
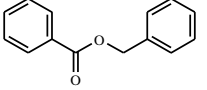
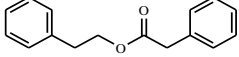
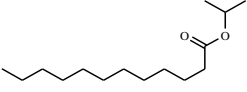
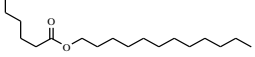
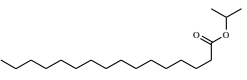
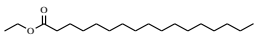
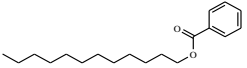
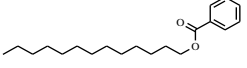
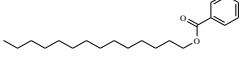
### Amino acids degradation products and miscellaneous acids

2-Hydroxypropanoic acid		C3H6O3	90.0317	91.0395
3-Methyl-2-oxopentanoic acid		C6H10O3	130.0630	131.0708
4-Methyl-2-oxopentanoic acid		C6H10O3	130.0630	131.0708
4-Ethylheptanoic acid		C9H18O2	158.1307	159.1385
Phenylacetic acid		C8H8O2	136.0524	137.0603
4-Ethyl-octanoic acid ('goat acid')		C10H20O2	172.1463	173.1542
8-Hydroxyoctanoic acid		C8H16O3	160.1099	161.1178
Octanedioic acid (suberic acid)		C8H14O4	174.0892	175.097
9-Hydroxynonanoic acid		C9H18O3	174.1256	175.1334
(4-Hydroxyphenyl)acetic acid		C8H8O3	152.0473	153.0552
Nonanedioic acid (azelaic acid)		C9H16O4	188.1049	189.1127
2-Ethylhexanoic acid		C8H16O2	144.115	145.1229
2-Piperidinone		C5H9NO	99.0684	100.0762
2-Methylhexanoic acid		C7H14O2	130.0994	131.1072
2-Methylheptanoic acid		C8H16O2	144.115	145.1229
2-Methyloctanoic acid		C9H18O2	158.1307	159.1385

2-Methylnonanoic acid		C <sub>10</sub> H <sub>20</sub> O <sub>2</sub>	172.1463	173.1542
2-Methyldecanoic acid		C <sub>11</sub> H <sub>22</sub> O <sub>2</sub>	186.162	187.1698
8-Methylundecanoic acid		C <sub>12</sub> H <sub>24</sub> O <sub>2</sub>	200.1776	201.1855
9-Methyldodecanoic acid		C <sub>13</sub> H <sub>26</sub> O <sub>2</sub>	214.1933	215.2011
10-Methyltridecanoic acid		C <sub>14</sub> H <sub>28</sub> O <sub>2</sub>	228.2089	229.2168
Isovaleric acid		C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	102.0681	103.0759
3-Methylhexanoic acid		C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	130.0994	131.1072
4-Ethylpentanoic acid		C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	130.0994	131.1072
4-Ethylnonanoic acid		C <sub>11</sub> H <sub>22</sub> O <sub>2</sub>	186.162	187.1698
4-Ethyldecanoic acid		C <sub>12</sub> H <sub>24</sub> O <sub>2</sub>	200.1776	201.1855
Propanoic acid		C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	74.0368	75.0446
Hexanoic acid		C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	116.0837	117.0916
Benzoic acid		C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	122.0368	123.0446
Dodecanoic acid		C <sub>12</sub> H <sub>24</sub> O <sub>2</sub>	200.1776	201.1855
Tetradecanoic acid		C <sub>14</sub> H <sub>28</sub> O <sub>2</sub>	228.2089	229.2168
Pentadecanoic acid		C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>	242.2246	243.2324
Hexadecanoic acid		C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>	256.2402	257.2481
Heptadecanoic acid		C <sub>17</sub> H <sub>34</sub> O <sub>2</sub>	270.2559	271.2637
2-Methylhexadecanoic acid		C <sub>17</sub> H <sub>34</sub> O <sub>2</sub>	270.2559	271.2637
Octadecanoic acid		C <sub>18</sub> H <sub>36</sub> O <sub>2</sub>	284.2715	285.2794


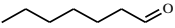

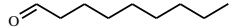
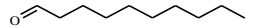
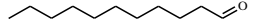

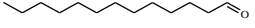
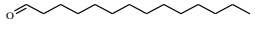

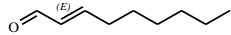
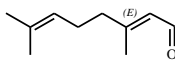
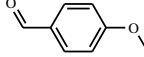
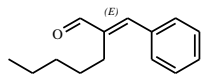
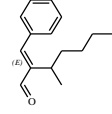
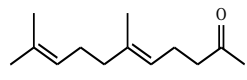
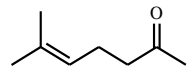
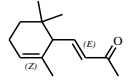
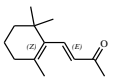
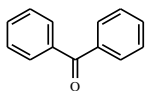
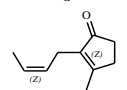
<i>n</i> -Heptanoic acid		C7H14O2	130.0994	131.1072
<i>n</i> -Octanoic acid		C8H16O2	144.115	145.1229
<i>n</i> -Nananoic acid		C9H18O2	158.1307	159.1385
<i>n</i> -Decanoic acid		C10H20O2	172.1463	173.1542
<i>n</i> -Undecanoic acid		C11H22O2	186.162	187.1698
<i>n</i> -Methyldodecanoic acid		C13H26O2	214.1933	215.2011
<i>n</i> -Methyltetradecanoic acid		C15H30O2	242.2246	243.2324
<b>Esters</b>				
7-Hexadecenoic acid methyl ester		C17H32O2	268.2402	269.2481
Acetic acid phenylmethyl ester		C9H10O2	150.0681	151.0759
2-Phenylethyl acetate		C10H12O2	164.0837	165.0916
Cyclopentanetridecanoic acid methyl ester		C19H36O2	296.2715	297.2794
Dodecanoic acid, 10-methyl, methyl ester		C14H28O2	228.2089	229.2168
Furancarboxylic acid methyl ester		C6H6O3	126.0317	127.0395
Hexanedioic acid dimethyl ester		C8H14O4	174.0892	175.0970
Methyl 9-methyltetradecanoate		C16H32O2	256.2402	257.2481
Propanedioic acid dimethyl ester		C5H8O4	132.0423	133.0501
Hexanoic acid methyl ester		C7H14O2	130.0994	131.1072
Octanoic acid methyl ester		C9H18O2	158.1307	159.1385
Nonanoic acid methyl ester		C10H20O2	172.1463	173.1542
Decanoic acid methyl ester		C11H22O2	186.162	187.1698

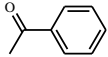
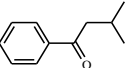
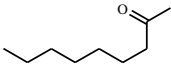
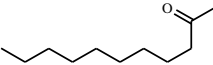
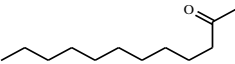
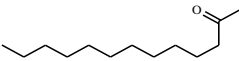
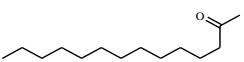
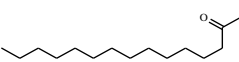
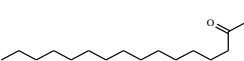

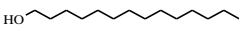
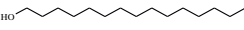
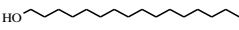
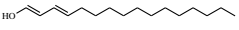
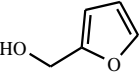
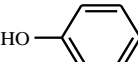
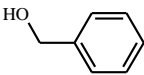
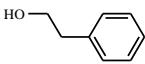
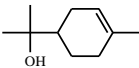
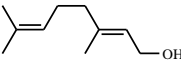
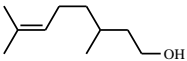
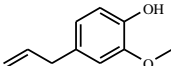
Undecanoic acid methyl ester		C12H24O2	200.1776	201.1855
Dodecanoic acid methyl ester		C13H26O2	214.1933	215.2011
Tridecanoic acid methyl ester		C14H28O2	228.2089	229.2168
Tetradecanoic acid methyl ester		C15H30O2	242.2246	243.2324
Pentadecanoic acid methyl ester		C16H32O2	256.2402	257.2481
Hexadecanoic acid methyl ester		C17H34O2	270.2559	271.2637
Heptadecanoic acid methylester		C18H36O2	284.2715	285.2794
9-Hexadecenoic acid methyl ester		C17H32O2	268.2402	269.2481
Terpinyl acetate		C12H20O2	196.1463	197.1542
Methyl-N-methylantranilate		C9H11NO2	165.079	166.0868
2-Hexyl 2-pentenoate		C11H20O2	184.1463	185.1542
E-Cinnamyl acetate		C11H12O2	176.0837	177.0916
$\alpha$ -Trichloromethyl-benzyl acetate		C10H9Cl3O2	265.9668	266.9746
Isoeugenol acetate		C12H14O3	206.0943	207.1021
Dihydromyrcenol acetate		C12H20O2	196.1463	197.1542
Neryl acetate		C12H20O2	196.1463	197.1542
Geranyl acetate		C12H20O2	196.1463	197.1542
Citronellol acetate		C12H22O2	198.162	199.1698
Methylcis-dihydrojasmonate		C12H19O3	211.1334	212.1412

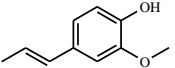
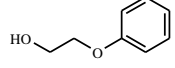


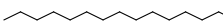





Pentyl salicylate		C12H16O3	208.1099	209.1178
Methyl trans-jasmonate		C12H18O3	210.1256	211.1334
1-Hexenyl salicylate		C13H16O3	220.1099	221.1178
1-Hexyl salicylate		C13H18O3	222.1256	223.1334
2-Ethylhexyl salicylate		C15H22O3	250.1569	251.1647
Ethyl tetradecanoate		C16H32O2	256.2402	257.2481
Ethyl pentadecanoate		C17H34O2	270.2559	271.2637
Ethyl hexadecanoate		C18H36O2	284.2715	285.2794
Benzyl benzoate		C14H12O2	212.0837	213.0916
2-phenylethyl phenylacetate		C16H16O2	240.1150	241.1229
Isopropyl dodecanoate		C15H30O2	242.2246	243.2324
Dodecyl hexanoate		C18H36O2	284.2715	285.2794
Hexadecanoic acid isopropyl ester		C19H38O2	298.2872	299.2950
Ethyl heptadecanoate		C19H38O2	298.2872	299.2950
Dodecyl benzoate		C19H30O2	290.2246	291.2324
Tridecyl benzoate		C20H32O2	304.2402	305.2481
Tetradecyl benzoate		C21H34O2	318.2559	319.2637


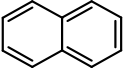

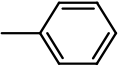
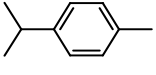
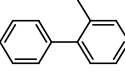
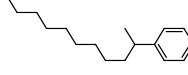
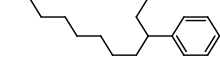
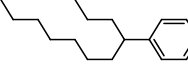
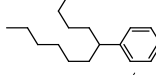

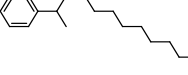
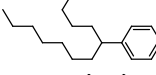
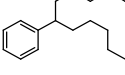
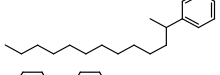
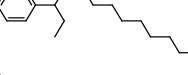
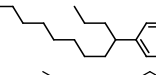
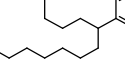
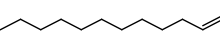
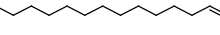
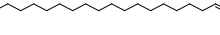
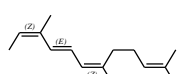


Decyl octanoate		C18H36O2	284.2715	285.2794
Dodecyl octanoate		C20H40O2	312.3028	313.3107
Tetradecyl octanoate		C22H44O2	340.3341	341.3420
2-Ethylhexyl 4-methoxycinnamate		C18H26O3	290.1882	291.1960
1-Octyl 4-methoxycinnamate		C18H26O3	290.1882	291.1960
2-Ethyl-hexyl 4-methoxycinnamate		C18H26O3	290.1882	291.1960
Isooctanedioldibutyrate		C16H30O4	286.2144	287.2222
<b>Amines</b>				
2-Pentylpyrrole		C9H15N	137.1204	138.1283
2-Phenoxyethylmethanamine		C9H13NO	151.0997	152.1075
Nicotine		C10H14N2	162.1157	163.1235
4-Sec-butylaniline		C10H15N	149.1204	150.1283
N,N-Dimethyl-1-dodecylamine		C14H31N	213.2457	214.2535
N,N-Dimethyl-1-hexadecylamine		C18H39N	269.3083	270.3161
N,N-Dimethyl-1-octadecylamine		C20H43N	297.3396	298.3474
<b>Amides</b>				
Methyl N,N-diethylthiocarbamate		C6H13NOS	147.0718	148.0796
n-Propylbenzamide		C10H13NO	163.0997	164.1075
Hydroxy acetanilide		C8H9NO2	151.0633	152.0712
<b>Aldehydes</b>				
2-Furancarboxaldehyde		C5H4O2	96.0211	97.029
Benzaldehyde		C7H6O	106.0419	107.0497

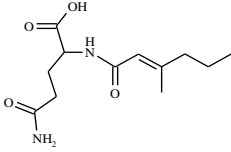
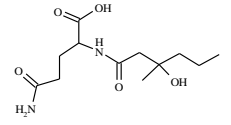
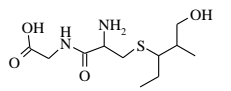
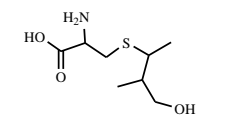
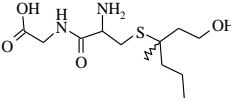
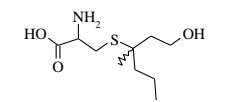
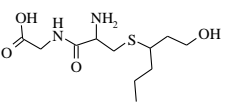
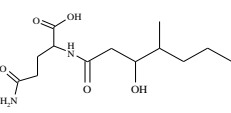
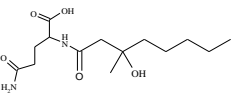
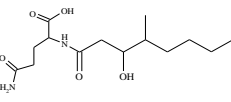
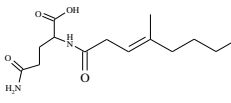
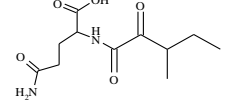
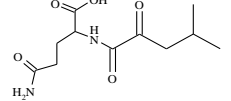
Hexanal		C <sub>6</sub> H <sub>12</sub> O	100.0888	101.0966
Heptanal		C <sub>7</sub> H <sub>14</sub> O	114.1045	115.1123
Octanal		C <sub>8</sub> H <sub>16</sub> O	128.1201	129.1279
Nonanal		C <sub>9</sub> H <sub>18</sub> O	142.1358	143.1436
Decanal		C <sub>10</sub> H <sub>20</sub> O	156.1514	157.1592
Undecanal		C <sub>11</sub> H <sub>22</sub> O	170.1671	171.1749
Dodecanal		C <sub>12</sub> H <sub>24</sub> O	184.1827	185.1905
Tridecanal		C <sub>13</sub> H <sub>26</sub> O	198.1984	199.2062
Tetradecanal		C <sub>14</sub> H <sub>28</sub> O	212.214	213.2218
Hexadecanal		C <sub>16</sub> H <sub>32</sub> O	240.2453	241.2531
(E)-2-Nonenal		C <sub>9</sub> H <sub>16</sub> O	140.1201	141.1279
Geranial		C <sub>10</sub> H <sub>16</sub> O	152.1201	153.1279
p-Anisaldehyde		C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	136.0524	137.0524
Pentylcinnamaldehyde		C <sub>14</sub> H <sub>18</sub> O	202.1358	203.1436
E-2-Hexylcinnamaldehyde		C <sub>15</sub> H <sub>20</sub> O	216.1514	217.1592
<b>Ketones</b>				
6,10-Dimethyl-5,9-undecadien-2-one		C <sub>13</sub> H <sub>22</sub> O	194.1671	195.1749
6-Methyl-5-hepten-2-one		C <sub>8</sub> H <sub>14</sub> O	126.1045	127.1123
α-Ionone		C <sub>13</sub> H <sub>20</sub> O	192.1514	193.1592
β-Ionone		C <sub>13</sub> H <sub>20</sub> O	192.1514	193.1592
Benzophenone		C <sub>13</sub> H <sub>10</sub> O	182.0732	183.0810
Jasmone		C <sub>11</sub> H <sub>16</sub> O	164.1201	165.1279

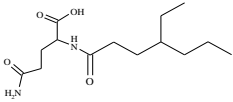
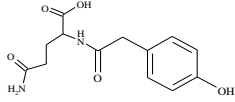
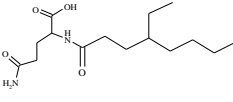
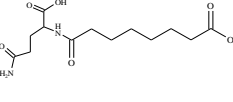
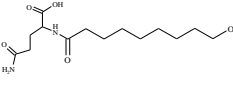
Acetophenone		C8H8O	120.0575	121.0653
Isopropylacetophenone		C11H14O	162.1045	163.1045
2-Nonanone		C9H18O	142.1358	143.1436
2-Undecanone		C11H22O	170.1671	171.1749
2-Dodecanone		C12H24O	184.1827	185.1905
2-Tridecanone		C13H26O	198.1984	199.2062
2-Tetradecanone		C14H28O	212.2140	213.2218
2-Pentadecanone		C15H30O	226.2297	227.2375
2-Hexadecanone		C16H32O	240.2453	241.2531
<b>Alcohols</b>				
Tridecan-1-ol		C13H28O	200.2140	201.2218
<i>n</i> -Tetradecanol		C14H30O	214.2297	215.2375
Pentadecanol		C15H32O	228.2453	229.2531
<i>n</i> -Hexadecanol		C16H34O	242.2610	243.2688
$\alpha$ Hexadecadienol		C16H30O	238.2297	239.2375
2-Furanmethanol		C5H6O2	98.0368	99.0446
Phenol		C6H6O	94.0419	95.0497
Benzyl Alcohol		C7H8O	108.0575	109.0653
2-Phenylethanol		C8H10O	122.0732	123.0810
<i>p</i> -Menth-1-en-8-ol		C10H18O	154.1358	155.1436
Geraniol		C10H18O	154.1358	155.1436
Citronellol		C10H20O	156.1514	157.1592
Eugenol		C10H12O2	164.0837	165.0916

Isoeugenol		C10H12O2	164.0837	165.0916	
2-Phenoxyethanol		C8H10O2	138.0681	139.0759	
<b>Aliphatic/Aromatic</b>					
Nonane		C9H20	128.1565	129.1643	
Undecane		C11H24	156.1878	157.1956	
Dodecane		C12H26	170.2035	171.2113	
Tridecane		C13H28	184.2191	185.2269	
Tetradecane		C14H30	198.2348	199.2426	
Pentadecane		C15H32	212.2504	213.2582	
Hexadecane		C16H34	226.2661	227.2739	
Heptadecane		C17H36	240.2817	241.2895	
Octadecane		C18H38	254.2974	255.3052	
Nonadecane		C19H40	268.3130	269.3208	
Eicosane		C20H42	282.3287	283.3365	
Heneicosane		C21H44	296.3443	297.3521	
Docosane		C22H46	310.3600	311.3678	
Tricosane		C23H48	324.3756	325.3834	
Tetracosane		C24H50	338.3913	339.3991	
3-Methyloctadecane		C19H40	268.3130	269.3208	
3-Methylnonadecane		C20H42	282.3287	283.3365	
4-Methylpentadecane		C16H34	226.2661	227.2739	
Nonane, 1-chloro-		C9H19Cl	162.1175	163.1254	
Pyridine		C5H5N	79.0422	80.0500	

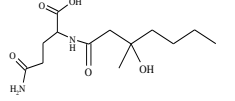
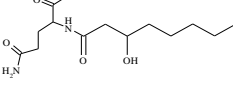
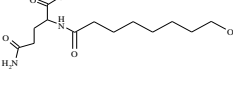
$\alpha$ -Pinene		C10H16	136.1252	137.1330
Naphthalene		C10H8	128.0626	129.0704
Cyclotetradecane		C14H28	196.2191	197.2269
Toluene		C7H8	92.0626	93.0704
p-Cymene		C10H14	134.1096	135.1174
Methyl biphenyl		C13H12	168.0939	169.1017
2-Phenylundecane		C17H28	232.2191	233.2269
3-Phenylundecane		C17H28	232.2191	233.2269
4-Phenylundecane		C17H28	232.2191	233.2269
5-Phenylundecane		C17H28	232.2191	233.2269
6-Phenylundecane		C17H28	232.2191	233.2269
2-Phenyldodecane		C18H30	246.2348	247.2426
5-Phenyldodecane		C18H30	246.2348	247.2426
6-Phenyldodecane		C18H30	246.2348	247.2426
2-Phenyltridecane		C19H32	260.2504	261.2582
3-Phenyltridecane		C19H32	260.2504	261.2582
4-Phenyltridecane		C19H32	260.2504	261.2582
6-Phenyltridecane		C19H32	260.2504	261.2582
1-Dodecene		C12H24	168.1878	169.1956
1-Tetradecene		C14H28	196.2191	197.2269
1-Nonadecene		C19H38	266.2974	267.3052
Farnesene		C15H24	204.1878	205.1956

**Precursors**

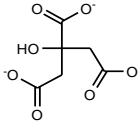
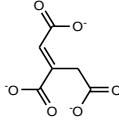
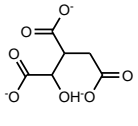
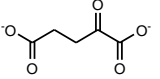
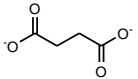
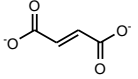
N- $\alpha$ -3-methylhex-2-enoyl-L-glutamine		C12H20N2O4	256.1423	257.1501
N- $\alpha$ -3-hydroxy-3-methylhexanoyl-L-glutamine		C12H22N2O5	274.1529	275.1607
S-[1-(2-hydroxy-1-methylethyl)-2-methylethyl]-L-cysteineglycine		C11H22N2O4S	278.1300	279.1379
S-[1-(2-hydroxy-1-methylethyl)-1-ethyl]-L-cysteine		C8H17NO3S	207.0929	208.1007
S-[1-(2-hydroxyethyl)-1-methylbutyl]-L-cysteineglycine		C12H24N2O4S	292.1457	293.1535
S-[1-(2-hydroxyethyl)-1-methylbutyl]-L-cystein		C10H21NO3S	235.1242	236.1320
S-[1-(2-hydroxyethyl)-butyl]-L-cysteineglycine		C11H22N2O4S	278.1300	279.1379
N- $\alpha$ -3-hydroxy-4-methylheptanoyl-L-glutamine		C13H24N2O5	288.1685	289.1763
N- $\alpha$ -3-hydroxy-3-methyloctanoyl-L-glutamine		C14H26N2O5	302.1842	303.1920
N- $\alpha$ -3-hydroxy-4-methyloctanoyl-L-glutamine		C14H26N2O5	302.1842	303.1920
N- $\alpha$ -4-methyl-3-oct-enoyl-L-glutamine		C14H24N2O4	284.1736	285.1814
N- $\alpha$ -3-methyl-2-oxopent-anoyl-L-glutamine		C11H18N2O5	258.1216	259.1294
N- $\alpha$ -4-methyl-2-oxopent-anoyl-L-glutamine		C11H18N2O5	258.1216	259.1294

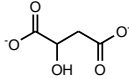
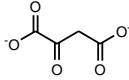

N- $\alpha$ -4-ethyl-hept-anoyl- L-glutamine		C14H26N2O4	286.1893	287.1971
N- $\alpha$ -4-hydroxyphenyl-acetyl- L-glutamine		C13H16N2O5	280.1059	281.1137
N- $\alpha$ -4-ethyl-oct-anoyl- L-glutamine		C15H28N2O4	300.2049	301.2127
N- $\alpha$ -7-carboxy-hept-anoyl- L-glutamine		C13H22N2O6	302.1478	303.1556
N- $\alpha$ -9-hydroxy- non-anoyl- L-glutamine		C14H26N2O5	302.1842	303.1920

### Hypothetical Precursors

N- $\alpha$ -3-hydroxy- 3-methylhept-anoyl- L-glutamine		C13H24N2O5	288.1685	289.1763
N- $\alpha$ -3-hydroxy-oct-anoyl- L-glutamine		C13H24N2O5	288.1685	289.1763
N- $\alpha$ -8-hydroxy-oct-anoyl- L-glutamine		C13H24N2O5	288.1685	289.1763

### TCA Cycle Intermediates

Citrate		C6H5O7 <sup>3-</sup>	189.0035	190.0114
Aconitate		C6H3O6 <sup>3-</sup>	170.9930	172.0008
Isocitrate		C6H5O7 <sup>3-</sup>	189.0035	190.0114
$\alpha$ -Ketoglutarate		C5H4O5 <sup>2-</sup>	144.0059	145.0137
Succinate		C4H4O4 <sup>2-</sup>	116.0110	117.0188
Fumarate		C4H4O2 <sup>2-</sup>	84.0211	85.0290

Malate		$C_4H_4O_5^{2-}$	132.0059	133.0137
Oxaloacetate		$C_4H_2O_5^{2-}$	129.9902	130.9980
Pyruvic acid		$C_3H_4O_3$	88.0160	89.0238