

Table S6

Index	Formula	Compounds	Class I	Class II	CAS	Cont1	Cont2	Cont3	DCM2	MyoC2	MyoC3	VIP	Fold_Change	
MEDN0097	C8H8O3	PhHydroxyphenyl Acetic Acid	—	Benzene acid substituted derivatives	—	156-38-7	92508	11740	8063.9	25454	9	9	1.076006671	0.226794963
MEDN0105	C26H45NO7S	Taurolithic acid	—	Bile acids	—	81-24-3	9	9	9	44992	17905	9	1.233334511	2296.518519
MEDN0198	C6H8O7	Citric Acid	—	Organic acid And Its derivatives	—	77-92-9	1233800	424350	1011800	4186000	3564500	2649200	1.543660243	3.895091668
MEDN0283	C4H8O3	2-Hydroxybutanoic Acid	2-___	Organic acid And Its derivatives	—	600-15-7	78565	9	9	87829	165740	200490	1.256626396	5.775536694
MEDN0334	C8H8O3	Mandelic Acid	—	Organic acid And Its derivatives	—	90-64-2	92509	11740	8063.9	25454	9	9	1.076006671	0.226794963
MEDN0352	C2H8NO4P	O-Phosphorylethanolamine	—	GP	—	1071-23-4	527990	307090	466430	2059500	664650	681400	1.26581867	2.61721782
MEDN0356	C28H44NO9P	Lysops 22:6	___22:6	GP	—	—	1654900	1485500	517810	213730	326790	698240	1.275622716	0.338624628
MEDN0368	C19H40NO7P	Lysope 14:0	___14:0	GP	—	—	6478.8	1894.3	1422	1181	473.9	851.64	1.22053116	0.255897336
MEDN0391	C22H32O2	DHA [4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoic acid]	—	Oxidized lipids	—	6217-54-5	6214400	7798900	3177000	2304900	2045800	2520800	1.433873493	0.399710317
MEDN0394	C20H36O2	Cis-11,14-Eicosadienoic Acid(C20:2)	___11,14-___	FA	—	2091-39-6	13514	14982	5146.9	7996.3	3254.3	2892.1	1.124902528	4.420376959
MEDN0396	C10H20O2	Capric Acid(C10:0)	—	FA	—	334-48-5	2318.4	2231.5	1831.9	2132.3	5075.3	5727.1	1.111892016	2.026810618
MEDN0399	C20H40O2	Arachidic Acid(C20:0)	—	FA	—	506-30-9	4699.8	2039.6	3110.9	21941	30077	35811	1.624858438	8.916378181
MEDN0502	C5H11O7P	2-Deoxyribose 1-Phosphate	2-___1-___	Carboxylic acids and derivatives	—	17210-42-3	1032600	500660	826840	145430	659280	334770	1.118569386	0.48281005
MEDN0506	C8H16NO9P	N-Acetylglucosamine 1-Phosphate	N-___1-___	Carboxylic acids and derivatives	—	6866-69-9	205130	92674	89775	1213900	315830	174580	1.225980695	4.397322868
MEDN0561	C11H16N2O8	N-Acetylaspartylglutamic acid	N-___	Amino acid and Its metabolomics	—	3106-85-2	36137	18086	19707	123780	142340	115130	1.628388015	5.156905181
MEDN0593	C4H6O5	D-Malic acid	D-(+)-___	Organic acid And Its derivatives	—	636-61-3	3268900	12392000	18235000	5988400	11896000	9542000	1.249540109	0.433359656
MEDN0598	C16H30O4	Hexadecanedioic acid	—	FA	—	505-54-4	14519	17686	24184	33283	45113	39464	1.511755496	2.09012396
MEDN0700	C20H34O5	5-IPF2_11 [8,11,13,15,17,19,21,23,25,27,29,31,33,35,37,39,41,43,45,47,49,51,53,55,57,59,61,63,65,67,69,71,73,75,77,79,81,83,85,87,89,91,93,95,97,99,101,103,105,107,109,111,113,115,117,119,121,123,125,127,129,131,133,135,137,139,141,143,145,147,149,151,153,155,157,159,161,163,165,167,169,171,173,175,177,179,181,183,185,187,189,191,193,195,197,199,201,203,205,207,209,211,213,215,217,219,221,223,225,227,229,231,233,235,237,239,241,243,245,247,249,251,253,255,257,259,261,263,265,267,269,271,273,275,277,279,281,283,285,287,289,291,293,295,297,299,301,303,305,307,309,311,313,315,317,319,321,323,325,327,329,331,333,335,337,339,341,343,345,347,349,351,353,355,357,359,361,363,365,367,369,371,373,375,377,379,381,383,385,387,389,391,393,395,397,399,401,403,405,407,409,411,413,415,417,419,421,423,425,427,429,431,433,435,437,439,441,443,445,447,449,451,453,455,457,459,461,463,465,467,469,471,473,475,477,479,481,483,485,487,489,491,493,495,497,499,501,503,505,507,509,511,513,515,517,519,521,523,525,527,529,531,533,535,537,539,541,543,545,547,549,551,553,555,557,559,561,563,565,567,569,571,573,575,577,579,581,583,585,587,589,591,593,595,597,599,601,603,605,607,609,611,613,615,617,619,621,623,625,627,629,631,633,635,637,639,641,643,645,647,649,651,653,655,657,659,661,663,665,667,669,671,673,675,677,679,681,683,685,687,689,691,693,695,697,699,701,703,705,707,709,711,713,715,717,719,721,723,725,727,729,731,733,735,737,739,741,743,745,747,749,751,753,755,757,759,761,763,765,767,769,771,773,775,777,779,781,783,785,787,789,791,793,795,797,799,801,803,805,807,809,811,813,815,817,819,821,823,825,827,829,831,833,835,837,839,841,843,845,847,849,851,853,855,857,859,861,863,865,867,869,871,873,875,877,879,881,883,885,887,889,891,893,895,897,899,901,903,905,907,909,911,913,915,917,919,921,923,925,927,929,931,933,935,937,939,941,943,945,947,949,951,953,955,957,959,961,963,965,967,969,971,973,975,977,979,981,983,985,987,989,991,993,995,997,999,1001,1003,1005,1007,1009,1011,1013,1015,1017,1019,1021,1023,1025,1027,1029,1031,1033,1035,1037,1039,1041,1043,1045,1047,1049,1051,1053,1055,1057,1059,1061,1063,1065,1067,1069,1071,1073,1075,1077,1079,1081,1083,1085,1087,1089,1091,1093,1095,1097,1099,1101,1103,1105,1107,1109,1111,1113,1115,1117,1119,1121,1123,1125,1127,1129,1131,1133,1135,1137,1139,1141,1143,1145,1147,1149,1151,1153,1155,1157,1159,1161,1163,1165,1167,1169,1171,1173,1175,1177,1179,1181,1183,1185,1187,1189,1191,1193,1195,1197,1199,1201,1203,1205,1207,1209,1211,1213,1215,1217,1219,1221,1223,1225,1227,1229,1231,1233,1235,1237,1239,1241,1243,1245,1247,1249,1251,1253,1255,1257,1259,1261,1263,1265,1267,1269,1271,1273,1275,1277,1279,1281,1283,1285,1287,1289,1291,1293,1295,1297,1299,1301,1303,1305,1307,1309,1311,1313,1315,1317,1319,1321,1323,1325,1327,1329,1331,1333,1335,1337,1339,1341,1343,1345,1347,1349,1351,1353,1355,1357,1359,1361,1363,1365,1367,1369,1371,1373,1375,1377,1379,1381,1383,1385,1387,1389,1391,1393,1395,1397,1399,1401,1403,1405,1407,1409,1411,1413,1415,1417,1419,1421,1423,1425,1427,1429,1431,1433,1435,1437,1439,1441,1443,1445,1447,1449,1451,1453,1455,1457,1459,1461,1463,1465,1467,1469,1471,1473,1475,1477,1479,1481,1483,1485,1487,1489,1491,1493,1495,1497,1499,1501,1503,1505,1507,1509,1511,1513,1515,1517,1519,1521,1523,1525,1527,1529,1531,1533,1535,1537,1539,1541,1543,1545,1547,1549,1551,1553,1555,1557,1559,1561,1563,1565,1567,1569,1571,1573,1575,1577,1579,1581,1583,1585,1587,1589,1591,1593,1595,1597,1599,1601,1603,1605,1607,1609,1611,1613,1615,1617,1619,1621,1623,1625,1627,1629,1631,1633,1635,1637,1639,1641,1643,1645,1647,1649,1651,1653,1655,1657,1659,1661,1663,1665,1667,1669,1671,1673,1675,1677,1679,1681,1683,1685,1687,1689,1691,1693,1695,1697,1699,1701,1703,1705,1707,1709,1711,1713,1715,1717,1719,1721,1723,1725,1727,1729,1731,1733,1735,1737,1739,1741,1743,1745,1747,1749,1751,1753,1755,1757,1759,1761,1763,1765,1767,1769,1771,1773,1775,1777,1779,1781,1783,1785,1787,1789,1791,1793,1795,1797,1799,1801,1803,1805,1807,1809,1811,1813,1815,1817,1819,1821,1823,1825,1827,1829,1831,1833,1835,1837,1839,1841,1843,1845,1847,1849,1851,1853,1855,1857,1859,1861,1863,1865,1867,1869,1871,1873,1875,1877,1879,1881,1883,1885,1887,1889,1891,1893,1895,1897,1899,1901,1903,1905,1907,1909,1911,1913,1915,1917,1919,1921,1923,1925,1927,1929,1931,1933,1935,1937,1939,1941,1943,1945,1947,1949,1951,1953,1955,1957,1959,1961,1963,1965,1967,1969,1971,1973,1975,1977,1979,1981,1983,1985,1987,1989,1991,1993,1995,1997,1999,2001,2003,2005,2007,2009,2011,2013,2015,2017,2019,2021,2023,2025,2027,2029,2031,2033,2035,2037,2039,2041,2043,2045,2047,2049,2051,2053,2055,2057,2059,2061,2063,2065,2067,2069,2071,2073,2075,2077,2079,2081,2083,2085,2087,2089,2091,2093,2095,2097,2099,2101,2103,2105,2107,2109,2111,2113,2115,2117,2119,2121,2123,2125,2127,2129,2131,2133,2135,2137,2139,2141,2143,2145,2147,2149,2151,2153,2155,2157,2159,2161,2163,2165,2167,2169,2171,2173,2175,2177,2179,2181,2183,2185,2187,2189,2191,2193,2195,2197,2199,2201,2203,2205,2207,2209,2211,2213,2215,2217,2219,2221,2223,22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1.961657282	up	HMDB0000094	SMP0000057;SMP0000466;SMP0000546;SMP0000547;SMP0000548;SMP0000549;SMP0000550;SMP0000551;SMP0000654;SMP0002231;SMP0002292;SMP0002295;SMP0002298;SMP0002358;SMP0002359;SMP00083
2.529955016	up	HMDB0000008	SMP0000016;SMP0000198;SMP0000201;SMP0000502
-2.140539496	down	HMDB0000703	--
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-1.965262964	down	--	--
-1.322973284	down	HMDB0002183	SMP0000018
-1.250244497	down	HMDB0000500	--
1.019211292	up	HMDB0000511	SMP0000456
3.156457809	up	HMDB0002212	--
-1.050472387	down	HMDB0001351	SMP0000050;SMP0000031;SMP0000144;SMP0000167;SMP0000365;SMP0000364;SMP0000203;SMP0000220;SMP0000210;SMP0000168;SMP0000046;SMP0000172;SMP0000219;SMP0000178;SMP0000202;SMP0000
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-1.206363243	down	HMDB0001518	--
1.053586508	up	HMDB0000672	--
12.13852767	up	--	--
11.01291418	up	--	--
2.229115163	up	--	--
-11.0632952	down	--	--
-2.040870722	down	--	--
-1.330490962	down	--	--
2.696501975	up	--	--
-1.322973284	down	--	--
-2.400446589	down	HMDB0001975	--
-4.822273627	down	--	--
1.251656739	up	HMDB0001057	--
-1.237231707	down	--	--
-1.670199535	down	--	--
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-2.725640265	down	--	--
-2.513737684	down	--	--
-3.629404396	down	--	--
-3.629404396	down	--	--
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1.181726646	up	HMDB0000043	SMP0000123;SMP0000033;SMP0000031;SMP0000314;SMP0000317;SMP0000316;SMP0000222;SMP0000340;SMP0000221;SMP0000004;SMP0000242;SMP0000179;SMP0000244;SMP0000223;SMP0000484;SMP0000485;SMP0000
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1.218657101	up	HMDB0001414	SMP0000445;SMP0000033;SMP0000177;SMP0000341;SMP0000214;SMP0000222;SMP0000340;SMP0000221;SMP00000570
3.659882808	up	HMDB0000403	--
1.863712932	up	HMDB0000068	SMP0000012;SMP0000169;SMP0000006;SMP0000190;SMP0000218;SMP0000429;SMP0000494;SMP0000497;SMP0000498;SMP0000053;SMP0000661
2.033569336	up	HMDB0000763	SMP0000063
2.186124017	up	HMDB0000681	--
-1.734166738	down	HMDB0010379	SMP0000075;SMP0000353;SMP0000077;SMP0000083;SMP0000084;SMP0000085;SMP0000086;SMP0000087;SMP0000093;SMP0000094;SMP0000096;SMP0000098;SMP0000101;SMP0000102;SMP0000104;SMP0000
-1.960962573	down	HMDB0010383	--
-1.721617559	down	HMDB0010385	--
-2.337902118	down	HMDB0010386	--
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-1.101199151	down	HMDB0002660	--
1.123726213	up	HMDB0000157	--
-1.326180608	down	HMDB0000453	--
-1.07528858	down	HMDB0000895	SMP0000025;SMP0000225;SMP0000226;SMP0000227;SMP0000228;SMP0000229;SMP0000230;SMP0000231;SMP0000232;SMP0000233;SMP0000248;SMP0000589;SMP0000734;SMP0000735;SMP0000736;SMP00051
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-1.204042961	down	--	--
-1.66229786	down	--	--
-1.912411146	down	HMDB0000138	SMP0000035;SMP0000314;SMP0000318;SMP0000317;SMP0000316;SMP0000315;SMP0000720
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2.023476035	up	HMDB0000234	SMP0000068;SMP0000356;SMP0000565;SMP0000406
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-1.146623363	down	HMDB0001999	SMP0000018
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-1.282323847	down	--	--
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6.016960941	up	HMDB0042560	--
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3.247893647	up	HMDB0010468	--
5.111072601	up	HMDB0049399	--
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4.207628115	up	HMDB0048609	--
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4.211917009	up	--	--
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