

Table 1: Acyl-CoA Mass List

Isotopologue	Precursor Formula [M]	Precursor Ion [M+H] ⁺	Product Ion [M+H-507] ⁺
Succinyl-CoA	C25H40N7O19P3S	868.1385	361.1428
Succinyl-CoA-M1	[13]C1C24H40N7O19P3S	869.1419	362.1461
Succinyl-CoA-M2	[13]C2C23H40N7O19P3S	870.1452	363.1495
Succinyl-CoA-M3	[13]C3C22H40N7O19P3S	871.1486	364.1528
Succinyl-CoA-M4	[13]C4C21H40N7O19P3S	872.1520	365.1562
Succinyl-CoA-M5	[13]C5C20H40N7O19P3S	873.1553	366.1596
Succinyl-CoA-M6	[13]C6C19H40N7O19P3S	874.1587	367.1629
Succinyl-CoA-M7	[13]C7C18H40N7O19P3S	875.1620	368.1663
Acetyl-CoA	C23H38N7O17P3S	810.1331	303.1373
Acetyl-CoA-M1	[13]C1C22H38N7O17P3S	811.1364	304.1407
Acetyl-CoA-M2	[13]C2C21H38N7O17P3S	812.1398	305.1440
Acetyl-CoA-M3	[13]C3C20H38N7O17P3S	813.1431	306.1474
Acetyl-CoA-M4	[13]C4C19H38N7O17P3S	814.1465	307.1507
Acetyl-CoA-M5	[13]C5C18H38N7O17P3S	815.1498	308.1541
Propionyl-CoA	C24H40N7O17P3S	824.1487	317.1530
Propionyl-CoA-M1	[13]C1C23H40N7O17P3S	825.1521	318.1563
Propionyl-CoA-M2	[13]C2C22H40N7O17P3S	826.1554	319.1488
Propionyl-CoA-M3	[13]C3C20H40N7O17P3S	827.1588	320.1521
Propionyl-CoA-M4	[13]C4C19H40N7O17P3S	828.1621	321.1555
Propionyl-CoA-M5	[13]C5C18H40N7O17P3S	829.1655	322.1564
3HMG-CoA*	C27H44N7O20P3S	912.1647	405.1690
3HMG-CoA-M1	[13]C1C26H44N7O20P3S	913.1681	406.1724
3HMG-CoA-M2	[13]C2C25H44N7O20P3S	914.1715	407.1757
3HMG-CoA-M3	[13]C3C24H44N7O20P3S	915.1748	408.1791
3HMG-CoA-M4	[13]C4C23H44N7O20P3S	916.1782	409.1824
3HMG-CoA-M5	[13]C5C22H44N7O20P3S	917.1815	410.1858
3HMG-CoA-M6	[13]C6C21H44N7O20P3S	918.1849	411.1891
3HMG-CoA-M7	[13]C7C20H44N7O20P3S	919.1882	412.1925
3HMG-CoA-M8	[13]C8C19H44N7O20P3S	920.1916	413.1958
3HMG-CoA-M9	[13]C9C18H44N7O20P3S	921.1949	414.1992
3H(I)B-CoA**	C25H42N7O18P3S	854.1593	347.1635
3H(I)B -CoA-M1	[13]C1C24H42N7O18P3S	855.1626	348.1669
3H(I)B -CoA-M2	[13]C2C23H42N7O18P3S	856.1660	349.1702
3H(I)B -CoA-M3	[13]C3C22H42N7O18P3S	857.1693	350.1736
3H(I)B -CoA-M4	[13]C4C21H42N7O18P3S	858.1727	351.1769
3H(I)B -CoA-M5	[13]C5C20H42N7O18P3S	859.1760	352.1803
3H(I)B -CoA-M6	[13]C6C19H42N7O18P3S	860.1794	353.1836
3H(I)B -CoA-M7	[13]C7C18H42N7O18P3S	861.1827	354.1870
[Iso]Butyryl-CoA	C25H42N7O17P3S	838.1644	331.1686
[Iso]Butyryl-CoA-M1	[13]C1C24H42N7O17P3S	839.1677	332.1720
[Iso]Butyryl-CoA-M2	[13]C2C23H42N7O17P3S	840.1711	333.1753
[Iso]Butyryl-CoA-M3	[13]C3C22H42N7O17P3S	841.1744	334.1787
[Iso]Butyryl-CoA-M4	[13]C4C21H42N7O17P3S	842.1778	335.1820
[Iso]Butyryl-CoA-M5	[13]C5C20H42N7O17P3S	843.1811	336.1854
[Iso]Butyryl-CoA-M6	[13]C6C19H42N7O17P3S	844.1845	337.1887
[Iso]Butyryl-CoA-M7	[13]C7C18H42N7O17P3S	845.1878	338.1921
Acetyl-CoA SILEC	[13]C3C20H38[15]N1N6O17P3S	814.1401	307.1444
Acetyl-CoA SILEC-M1	[13]C4C19H38[15]N1N6O17P3S	815.1435	308.1478
Acetyl-CoA SILEC-M2	[13]C5C18H38[15]N1N6O17P3S	816.1469	309.1511
Acetyl-CoA SILEC-M3	[13]C6C17H38[15]N1N6O17P3S	817.1502	310.1545
Acetyl-CoA SILEC-M4	[13]C7C16H38[15]N1N6O17P3S	818.1536	311.1578
Acetyl-CoA SILEC-M5	[13]C8C15H38[15]N1N6O17P3S	819.1569	312.1612
Succinyl-CoA SILEC	[13]C3C22H40[15]N1N6O19P3S	872.1456	365.1499
Succinyl-CoA SILEC-M1	[13]C4C21H40[15]N1N6O19P3S	873.1490	366.1533
Succinyl-CoA SILEC-M2	[13]C5C20H40[15]N1N6O19P3S	874.1523	367.1566
Succinyl-CoA SILEC-M3	[13]C6C19H40[15]N1N6O19P3S	875.1557	368.1560
Succinyl-CoA SILEC-M4	[13]C7C18H40[15]N1N6O19P3S	876.1591	369.1633
Succinyl-CoA SILEC-M5	[13]C8C17H40[15]N1N6O19P3S	877.1624	370.1666
Succinyl-CoA SILEC-M6	[13]C9C16H40[15]N1N6O19P3S	878.1658	371.1700
Succinyl-CoA SILEC-M7	[13]C10C15H40[15]N1N6O19P3S	879.1691	372.1734

*HMG-CoA (3-hydroxymethylglutaryl-CoA), **3H(I)B-CoA (3-hydroxybutyrate-CoA/3-hydroxyisobutyrate-CoA)

Table 2: TCA Cycle Mass List

Isotopologue	Formula [M]	Precursor Ion [M-H]-
Glutamine	C5H10N2O3	145.0608
[13]C1-glutamine	[13]C1C4H10N2O3	146.0641
[13]C2-glutamine	[13]C2C3H10N2O3	147.0675
[13]C3-glutamine	[13]C3C2H10N2O3	148.0708
[13]C4-glutamine	[13]C4C1H10N2O3	149.0742
[13]C5-glutamine	[13]C5H10N2O3	150.0775
[15]N1-glutamine	C5H10[15]N1N1O3	146.0589
[13]C1[15]N1-glutamine	[13]C1C4H10[15]N1N1O3	147.0623
[13]C2[15]N1-glutamine	[13]C2C3H10[15]N1N1O3	148.0656
[13]C3[15]N1-glutamine	[13]C3C2H10[15]N1N1O3	149.0690
[13]C4[15]N1-glutamine	[13]C4C1H10[15]N1N1O3	150.0723
[13]C5[15]N1-glutamine	[13]C5H10[15]N1N1O3	151.0757
[15]N2-glutamine	C5H10[15]N2O3	147.0559
[13]C1[15]N2-glutamine	[13]C1C4H10[15]N2O3	148.0593
[13]C2[15]N2-glutamine	[13]C2C3H10[15]N2O3	149.0626
[13]C3[15]N2-glutamine	[13]C3C2H10[15]N2O3	150.0660
[13]C4[15]N2-glutamine	[13]C4C1H10[15]N2O3	151.0694
[13]C5[15]N2-glutamine	[13]C5H10[15]N2O3	152.0727
α -Ketoglutarate	C5H6O5	145.0142
[13]C1- α -Ketoglutarate	[13]C1C4H6O5	146.0176
[13]C2- α -Ketoglutarate	[13]C2C3H6O5	147.0185
[13]C3- α -Ketoglutarate	[13]C3C2H6O5	148.0218
[13]C4- α -Ketoglutarate	[13]C4C1H6O5	149.0227
[13]C5- α -Ketoglutarate	[13]C5H6O5	150.0261
Succinate	C4H5O4	117.0193
[13]C1-succinate	[13]C1C3H5O4	118.0227
[13]C2-succinate	[13]C2C2H5O4	119.0236
[13]C3-succinate	[13]C3C1H5O4	120.0269
[13]C4-succinate	[13]C4H5O4	121.0278
Malate	C4H6O5	133.0131
[13]C1-malate	[13]C1C3H6O5	134.0165
[13]C2-malate	[13]C2C2H6O5	135.0199
[13]C3-malate	[13]C3C1H6O5	136.0232
[13]C4-malate	[13]C4H6O5	137.0266
Citrate	C6H8O7	191.0197
[13]C1-citrate	[13]C1C5H8O7	192.0231
[13]C2-citrate	[13]C2C4H8O7	193.0240
[13]C3-citrate	[13]C3C3H8O7	194.0273
[13]C4-citrate	[13]C4C2H8O7	195.0331
[13]C5-citrate	[13]C5C1H8O7	196.0365
[13]C6-citrate	[13]C6H8O7	197.0374