

Supplementary Table S1. Inclusion list for the MS/MS data-dependent acquisition.

Transformation	Molecular formula	[M + H]⁺ (m/z)	[M - H]⁻ (m/z)
Parent (4-AcO-DiPT)	C ₁₈ H ₂₆ N ₂ O ₂	303.2067	301.1922
-2C-2H-O	C ₁₆ H ₂₄ N ₂ O	261.1961	259.1816
+O	C ₁₈ H ₂₆ N ₂ O ₃	319.2016	317.1871
-3C-6H	C ₁₅ H ₂₀ N ₂ O ₂	261.1598	259.1452
+O-2H	C ₁₈ H ₂₄ N ₂ O ₃	317.1860	315.1714
+4C+6H+5O	C ₂₂ H ₃₂ N ₂ O ₇	437.2282	435.2137
-2C-2H+2O+S	C ₁₆ H ₂₄ N ₂ O ₄ S	341.1530	339.1384
-2C-2H+2O+S	C ₁₆ H ₂₄ N ₂ O ₄ S	341.1530	339.1384
+2H+2O	C ₁₈ H ₂₈ N ₂ O ₄	337.2122	335.1976
-6C-13H-N+O	C ₁₂ H ₁₃ NO ₃	220.0968	218.0823
-6C-15H-N+O	C ₁₂ H ₁₁ NO ₃	218.0812	216.0666
+10C+17H+3N+7O+S	C ₂₈ H ₄₃ N ₅ O ₉ S	626.2854	624.2709
-6C-15H-N+2O	C ₁₂ H ₁₁ NO ₄	234.0761	232.0615
-2C-2H	C ₁₆ H ₂₄ N ₂ O ₂	277.1911	275.1765
-5C-8H-O	C ₁₃ H ₁₈ N ₂ O	219.1492	217.1346
+2O	C ₁₈ H ₂₆ N ₂ O ₄	335.1965	333.1820
+6C+8H+7O	C ₂₄ H ₃₄ N ₂ O ₉	495.2337	493.2192
+4O+S	C ₁₈ H ₂₆ N ₂ O ₆ S	399.1584	397.1439
-3C-6H+O	C ₁₅ H ₂₀ N ₂ O ₃	277.1547	275.1401
-6C-12H	C ₁₂ H ₁₄ N ₂ O ₂	219.1128	217.0983
+4C+6H+6O	C ₂₂ H ₃₂ N ₂ O ₈	453.2231	451.2086
-2C-2H+3O+S	C ₁₆ H ₂₄ N ₂ O ₅ S	357.1479	355.1333
-5C-8H	C ₁₃ H ₁₈ N ₂ O ₂	235.1441	233.1296
-2C-2H+O	C ₁₆ H ₂₄ N ₂ O ₃	293.1860	291.1714
-2C-4H	C ₁₆ H ₂₂ N ₂ O ₂	275.1754	273.1609
-8C-17H-N	C ₁₀ H ₉ NO ₂	176.0706	174.0561
-8C-17H-N+O	C ₁₀ H ₉ NO ₃	192.0655	190.0510
-3C-8H+O	C ₁₅ H ₁₈ N ₂ O ₃	275.1390	273.1245
-2C+O	C ₁₆ H ₂₆ N ₂ O ₃	295.2016	293.1871
+8C+15H+3N+6O+S	C ₂₆ H ₄₁ N ₅ O ₈ S	584.2749	582.2603
+C+6O	C ₁₉ H ₂₆ N ₂ O ₈	411.1762	409.1616
-5C-8H+3O+S	C ₁₃ H ₁₈ N ₂ O ₅ S	315.1009	313.0864
+4C+6H+7O	C ₂₂ H ₃₂ N ₂ O ₉	469.2181	467.2035
-2C-2H+4O+S	C ₁₆ H ₂₄ N ₂ O ₆ S	373.1428	371.1282
+C+5O	C ₁₉ H ₂₆ N ₂ O ₇	395.1813	393.1667
-8C-14H-O	C ₁₀ H ₁₂ N ₂ O	177.1022	175.0877
-5C-10H	C ₁₃ H ₁₆ N ₂ O ₂	233.1285	231.1139
-8C-16H	C ₁₀ H ₁₀ N ₂ O ₂	191.0815	189.0670
-5C-8H+2O+S	C ₁₃ H ₁₈ N ₂ O ₄ S	299.1060	297.0915

-2C-4H+O	C ₁₆ H ₂₂ N ₂ O ₃	291.1703	289.1558
+6C+8H+8O	C ₂₄ H ₃₄ N ₂ O ₁₀	511.2286	509.2141
+5O+S	C ₁₈ H ₂₆ N ₂ O ₇ S	415.1534	413.1388
-6C-14H+O	C ₁₂ H ₁₂ N ₂ O ₃	233.0921	231.0775
-2H+2O	C ₁₈ H ₂₄ N ₂ O ₄	333.1809	331.1663
-C-O	C ₁₇ H ₂₆ N ₂ O	275.2118	273.1972
+C+2H+O	C ₁₉ H ₂₈ N ₂ O ₃	333.2173	331.2027
-C	C ₁₇ H ₂₆ N ₂ O ₂	291.2067	289.1922
-2H	C ₁₈ H ₂₄ N ₂ O ₂	301.1911	299.1765
-2C-4H-O	C ₁₆ H ₂₂ N ₂ O	259.1805	257.1659
