

Table S1. Inclusion list used during liquid chromatography-high-resolution tandem mass spectrometry (LC-HRMS/MS) for dipyanone metabolite identification.

Dipyanone

Transformation	Elemental composition	[M+H] ⁺ <i>m/z</i>	[M-H] ⁻ <i>m/z</i>
Parent (Dipyanone)	<u>C₂₃H₂₉NO</u>	336.2322	334.2176
+O	C ₂₃ H ₂₉ NO ₂	352.2271	350.2126
+2O	C ₂₃ H ₂₉ NO ₃	368.2220	366.2075
+2H	C ₂₃ H ₃₁ NO	338.2478	336.2333
-2H+O	C ₂₃ H ₂₇ NO ₂	350.2115	348.1969
+2H+2O	C ₂₃ H ₃₁ NO ₃	370.2377	368.2231
+2H+O	C ₂₃ H ₃₁ NO ₂	354.2428	352.2282
-2H+2O	C ₂₃ H ₂₇ NO ₃	366.2064	364.1918
-2H	C ₂₃ H ₂₇ NO	334.2165	332.2020
+6C+10H+6O	C ₂₉ H ₃₉ NO ₇	514.2799	512.2654
+6C+8H+7O	C ₂₉ H ₃₇ NO ₈	528.2592	526.2446
+2H+S+3O	C ₂₃ H ₃₁ NO ₄ S	418.2047	416.1901
+S+4O	C ₂₃ H ₂₉ NO ₅ S	432.1839	430.1694
-4C-6H	C ₁₉ H ₂₃ NO	282.1852	280.1707
-4C-8H-1O	C ₁₉ H ₂₁ N	364.1747	262.1601
-1H+2O	C ₂₃ H ₂₈ NO ₂ +	350.2115	349.2042