

Supplementary Data 5. Analyte specific MS data of UHPLC-MS analysis in the positive ESI mode, showing the measured accurate mass, the mass deviation to the respective theoretical accurate mass, the molecular formula, and the retention time. Additionally, MS/MS data of the analytes are displayed (precursor ion and some major product ions).

Analyte	Measured accurate mass [Da]	Deviation of measured mass [ppm]	Molecular formula	Retention time [min]	Precursor ion (MS/MS analysis) [m/z]	Selected product ions (MS/MS analysis) [m/z]
Versicolorin B	341.0662	1.2	C ₁₈ H ₁₂ O ₇	22.9	341.1	323.1, 313.1, 299.0, 285.0
Dihydro-O-methylsterigmatocystin	341.1020	1.0	C ₁₉ H ₁₆ O ₆	19.7	341.1	326.1, 297.1, 285.1, 280.1
Dihydro-11-hydroxy-O-methylsterigmatocystin	357.0947	-1.6	C ₁₉ H ₁₆ O ₇	13.0	357.1	311.1, 299.1, 285.1, 269.0
Unknown metabolite	329.0659	1.0	C ₁₇ H ₁₂ O ₇ ^a	10.7	329.1	311.1, 301.1, 299.1, 273.0

^a this molecular mass is only postulated