

Figure S1. Comparison of the experimental fragmentation spectrum of betaine (top) with the spectrum from the mzCloud database (bottom).

RAWFILE(top): plasma_healthy_7_536_2_0h (F41) #672, RT=1.370 min, MS2, FTMS (+), (HCD, DDA, 286.1422@(20:40:80), +1)
 REFERENCE(bottom): mzCloud library, Piperine, C17 H19 N O3, MS2, FTMS, (HCD, 286.1438@(50:70:90))



Figure S2. Comparison of the experimental fragmentation spectrum of piperine (top) with the spectrum from the mzCloud database (bottom).

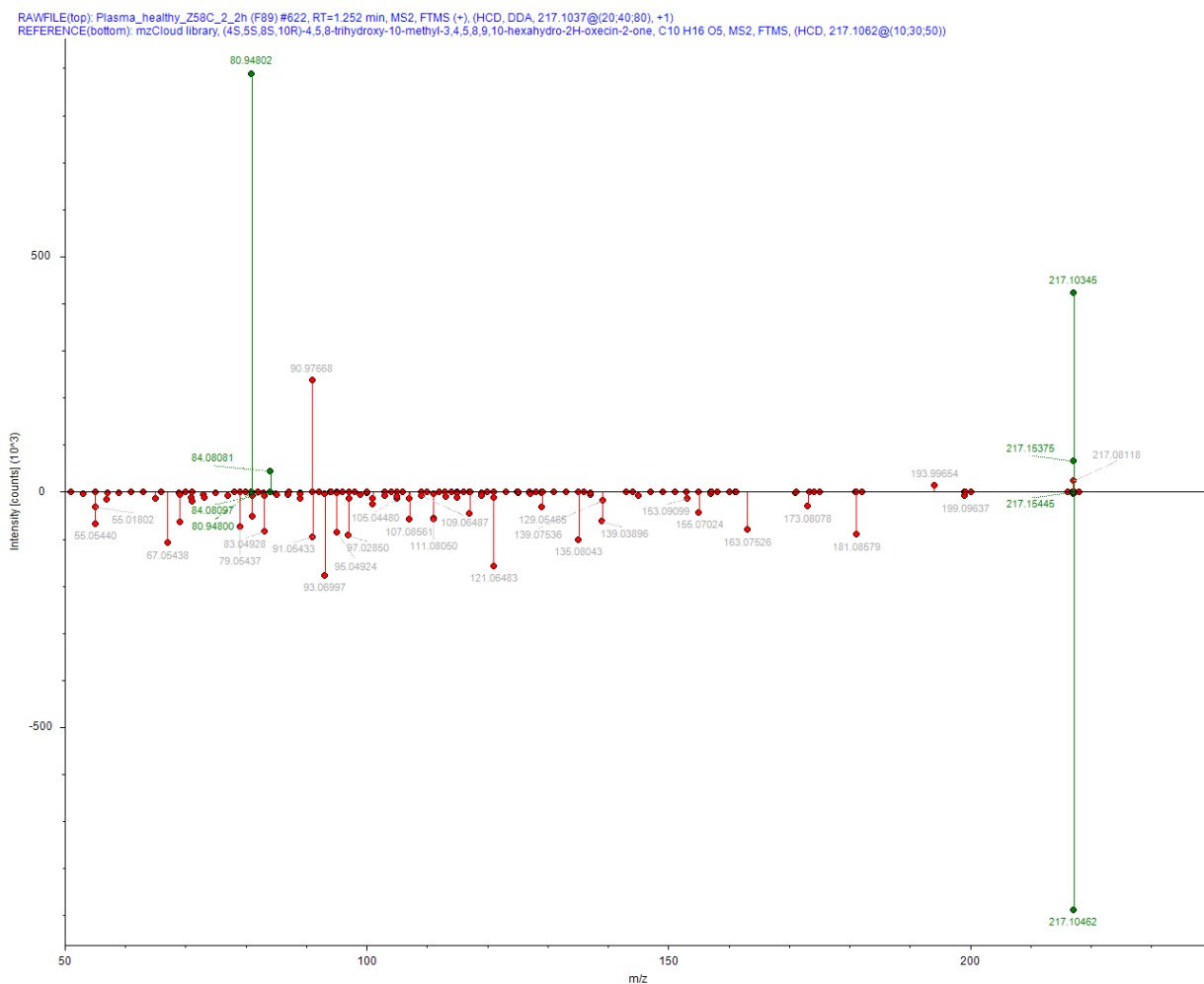


Figure S3. Comparison of the experimental fragmentation spectrum of (4S,5S,8S,10R)-4,5,8-trihydroxy-10-methyl-3,4,5,8,9,10-hexahydro-2H-oxecin-2-one (top) with the spectrum from the mzCloud database (bottom).

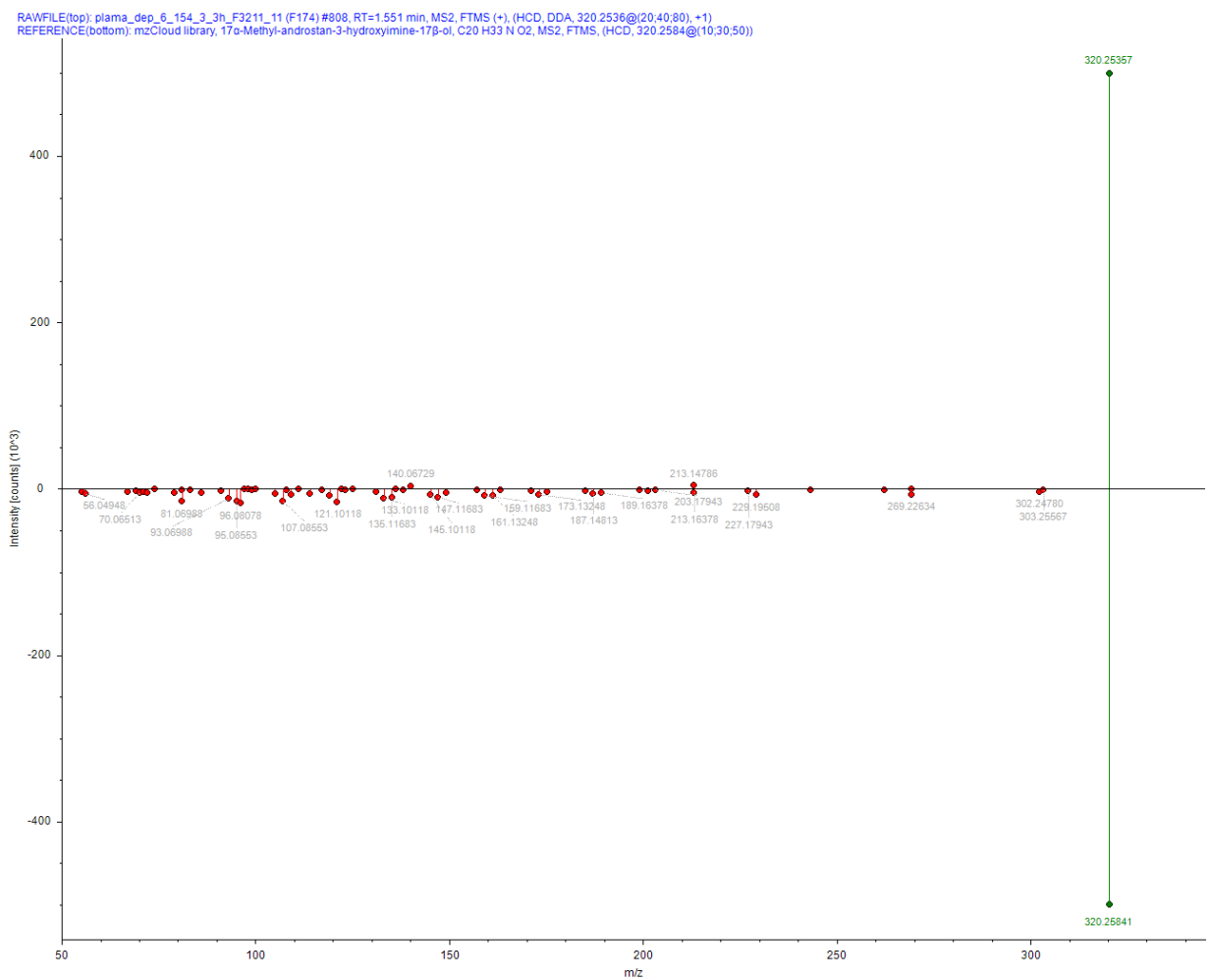


Figure S4. Comparison of the experimental fragmentation spectrum of 17 α -Methyl-androstan-3-hydroxyimine-17 β -ol (top) with the spectrum from the mzCloud database (bottom).

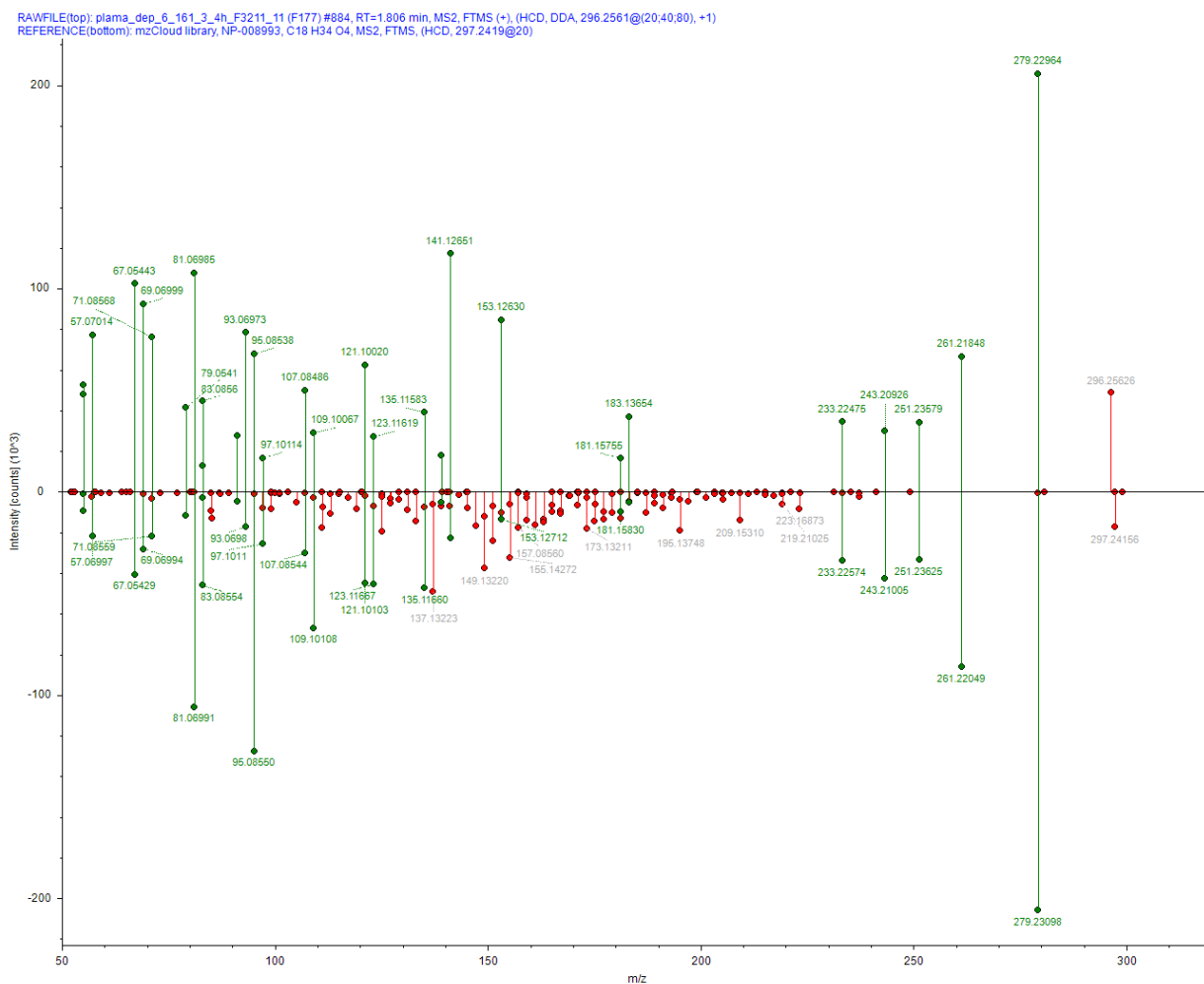


Figure S5. Comparison of the experimental fragmentation spectrum of (2E,4E)-N-(2-Hydroxy-2-methylpropyl)-2,4-tetradecadienamide (top) with the spectrum of NP-008993 from the mzCloud database (bottom).