

Supplementary Table S2. Data dependent settings for analysis on the LTQ-Orbitrap

Parent-ion mass	Neutral loss	Parent-ion structure	Parent molecule before oxidation/derivatisation
516.3948	79.04	C ^{4,x} -3-one 3-GP	Desmosterol/7-Dehydrocholesterol
518.4105	79.04	C ⁴ -3-one 3-GP	Cholesterol
520.4261	79.04	C-3-one 3-GP	3 β -Hydroxycholestane
532.3898	79.04	C ⁴ -3,x-dione 3-GP	Oxcholesterol
534.4054	79.04	C ⁴ -ol-3-one 3-GP	Hydroxycholesterol
536.4211	79.04	C-ol-3-one 3-GP	Dihydroxycholestane
546.3690	79.04	CA ^{4,x} -3-one 3-GP	3 β -Hydroxycholestadienoic acid
548.3847	79.04	CA ⁴ -3-one 3-GP	3 β -Hydroxycholestenoic acid
550.4003	79.04	C ⁴ -diol-3-one 3-GP	Dihydroxycholesterol
552.4160	79.04	C-diol-3-one 3-GP 5,6-seco-sterol/aldol 3-GP	Trihydroxycholestane 3 β -hydroxy-5-oxo-5,6-secocholestan-6-al
560.3483	79.04	CA ^{4,x,y} -ol-3-one 3-GP	Dihydroxycholestatrienoic acid
562.3639	79.04	CA ^{4,x} -ol-3-one 3-GP	Dihydroxycholestadienoic acid
564.3796	79.04	CA ⁴ -ol-3-one 3-GP	Dihydroxycholestenoic acid
566.3592	79.04	C ⁴ -triol-3-one 3-GP	Trihydroxycholesterol
568.4109	79.04	C-triol-3-one 3-GP	Tetrahydroxycholestane