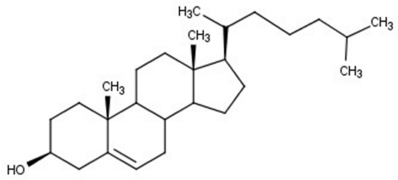
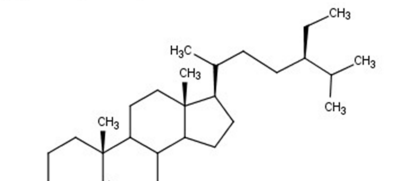
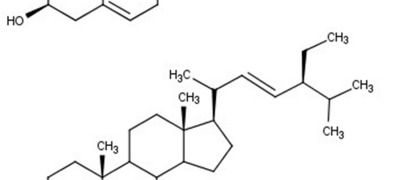
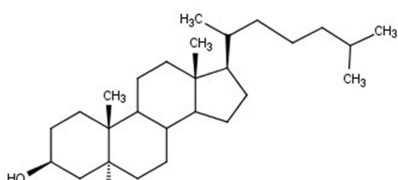
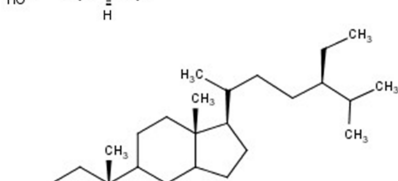
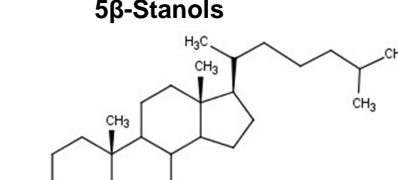
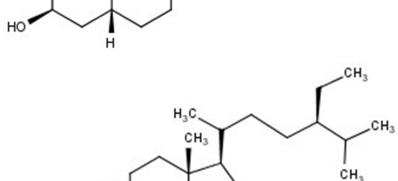


Supporting Information

“Steroid Biomarkers Revisited – Improved Source Identification of Faecal Remains in Archaeological Soil Material”

S4 Table. Studied compounds, molecular structures, retention times, and selected characteristic ion fragments.

Substance	Trivial name, molecular formula	Structure	Ret. time (min)	Characteristic ion fragments (m/z)
Δ^5-Sterols				
Cholest-5-en-3 β -ol	Cholesterol ^b C ₂₇ H ₄₆ O		41.7	329, 368, 458
5-Stigmasten-3 β -ol, 24-Ethyl-5-cholesten-3 β -ol	β -Sitosterol ^b C ₂₉ H ₅₀ O		50.5	129, 396, 486
Stigmasta-5,22-dien-3 β -ol	Stigmasterol ^b C ₂₉ H ₄₈ O		47.8	129, 394, 484
5α-Stanols				
5 α -Cholestan-3 β -ol	5 α -Cholestanol ^b (Dihydrocholesterol) C ₂₇ H ₄₈ O		42.2	445
24 α -Ethyl-5 α -cholestan-3 β -ol	5 α -Stigmasterol ^b (β -Sitostanol) C ₂₉ H ₅₂ O		51.0	215, 383, 473
5β-Stanols				
5 β -Cholestan-3 β -ol	Coprostanol ^b C ₂₇ H ₄₈ O		38.1	215, 257, 355, 370
24 β -Ethyl-5 β -cholestan-3 β -ol	5 β -stigmastanol ^{a,c} (24-Ethylcoprostanol) C ₂₉ H ₅₂ O		46.0	215, 257, 383, 398

^a according to the designation of the National Institute of Standards and Technology (NIST)

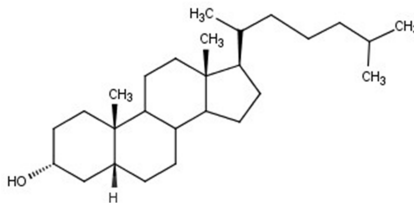
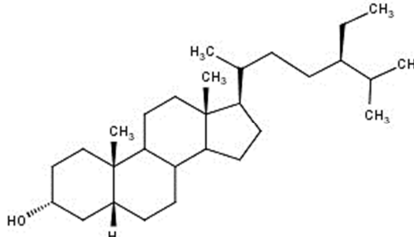
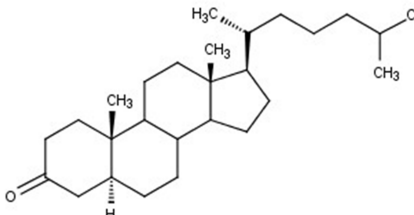
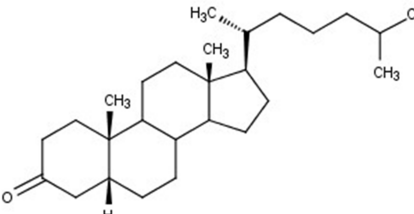
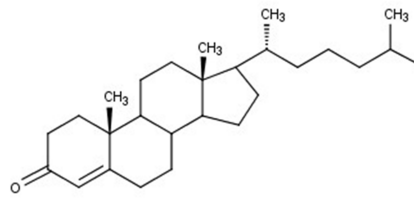
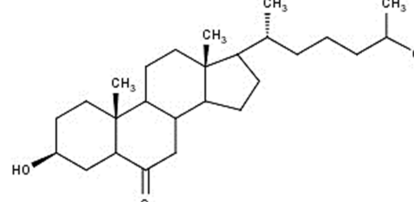
^b obtained from Sigma Aldrich (Taufkirchen, Germany)

^c obtained from Chiron AS (Trondheim, Norway; supplier: Campro Scientific, Berlin, Germany)

Supporting Information

“Steroid Biomarkers Revisited – Improved Source Identification of Faecal Remains in Archaeological Soil Material”

S4 Table (continuation). Studied compounds, molecular structures, retention times, and selected characteristic ion fragments.

Substance	Trivial name, molecular formula	Structure	Ret. time (min)	Characteristic ion fragments (m/z)
Epi-5β-stanols				
5 β -Cholestan-3 α -ol	Epicoprostanol ^b C ₂₇ H ₄₈ O		38.3	215, 257, 355, 370
24 β -Ethyl-5 β -cholestan-3 α -ol	Epi-5 β -stigmastanol ^c C ₂₉ H ₅₂ O		46.1	215, 257, 383, 398
Stanones				
5 α -Cholestan-3-one	Cholestanone ^b C ₂₇ H ₄₆ O		40.3	231, 316, 386
5 β -Cholestan-3-one	Coprostanone ^c C ₂₇ H ₄₆ O		42.4	386
	4-Cholesten-3-one ^b C ₂₇ H ₄₄ O		38.4	124, 229
3 β -Hydroxy-5 α -cholestan-6-one	6-Ketocholestanol ^b C ₂₇ H ₄₆ O ₂		46.0	445, 459, 474

^b obtained from Sigma Aldrich (Taufkirchen, Germany)

^c obtained from Chiron AS (Trondheim, Norway; supplier: Campro Scientific, Berlin, Germany)

Supporting Information

“Steroid Biomarkers Revisited – Improved Source Identification of Faecal Remains in Archaeological Soil Material”

S4 Table (continuation). Studied compounds, molecular structures, retention times, and selected characteristic ion fragments.

Substance	Trivial name, molecular formula	Structure	Ret. time (min)	Characteristic ion fragments (m/z)
Bile acids				
3 β -Hydroxy-5 β -cholanoic acid	Isolithocholic acid ^d (ILCA) C ₂₄ H ₄₀ O ₃		27.2	215, 257, 357
3 α -Hydroxy-5 β -cholanoic acid	Lithocholic acid ^b (LCA) C ₂₄ H ₄₀ O ₃		27.5	215, 257, 372
3 α ,12 α -Dihydroxy-5 β -cholanoic acid	Deoxycholic acid ^b (DCA) C ₂₄ H ₄₀ O ₄		29.2	255, 345, 370
3 α ,7 α -Dihydroxy-5 β -cholanoic acid	Chenodeoxycholic acid ^b (CDCA) C ₂₄ H ₄₀ O ₄		29.8	255, 355, 370
3 α ,6 α -Dihydroxy-5 β -cholanoic acid	Hyodeoxycholic acid ^b (HDCA) C ₂₄ H ₄₀ O ₄		30.3	255, 355, 370
3 α ,7 β -Dihydroxy-5 β -cholanoic acid	Ursodeoxycholic acid ^b (UDCA) C ₂₄ H ₄₀ O ₄		31.0	255, 370, 460

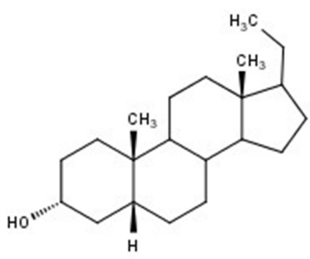
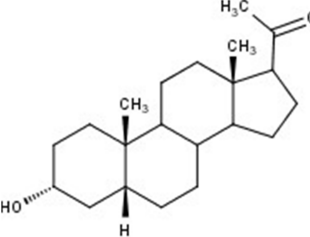
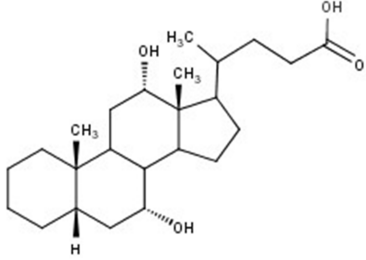
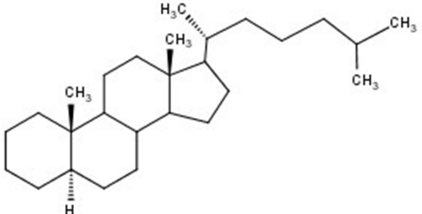
^b obtained from Sigma Aldrich (Taufkirchen, Germany)

^d obtained from Steraloids (Newport, RI, USA)

Supporting Information

“Steroid Biomarkers Revisited – Improved Source Identification of Faecal Remains in Archaeological Soil Material”

S4 Table (continuation). Studied compounds, molecular structures, retention times, and selected characteristic ion fragments.

Substance	Trivial name, molecular formula	Structure	Ret. time (min)	Characteristic ion fragments (m/z)
Internal standards				
5 β -Pregnan-3 α -ol	Desoxypregnanolone ^{d,e} C ₂₁ H ₃₆ O		23.4	286, 361
5 β -Pregnan-3 α -ol-20-one	Pregnanolone ^{d,e} C ₂₁ H ₃₄ O ₂		27.7	215, 300, 375
7 α ,12 α -Dihydroxy-5 β -cholanoic acid	Isodeoxycholic acid ^{d,e} (IDCA) C ₂₄ H ₄₀ O ₄		24.2	255, 355, 370
	5 α -cholestane ^{d,f} C ₂₇ H ₄₈		31.5 ^g / 20.1 ^h	217, 357, 372

^d obtained from Steraloids (Newport, RI, USA)

^e first internal standard (recovery standard)

^f second internal standard

^g measurement of sterols, stanols and stanones

^h measurement of bile acids