

Supporting Information

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

S8 Table. Sterol, stanol, and stanone contents of omnivore faeces (data from literature)

Steroid (trivial name)	Chicken ^{1x} (n=6)	Chicken ^{4x} (n=17)	Pig ^{1x} (n=6)	Pig ^{3x} (n=6)	Pig ^{4x} (n=26)	Pig ^{7c} (n=10)
Δ^5-Sterols ($\mu\text{g g}^{-1}$)						
Cholesterol	219 \pm 41 [‡]	5408 \pm 785 [‡]	127 \pm 27 [‡]	69 \pm 5 [‡]	3606 \pm 357 [‡]	11%
Stigmastanol	40 \pm 7	2872 \pm 380	0	7 \pm 1	1710 \pm 99	2%
β -Sitosterol	331 \pm 17	nd	139 \pm 10	151 \pm 11	nd	13.5%
5β-Stanols ($\mu\text{g g}^{-1}$)						
Coprostanol	12 \pm 7	1971 \pm 437	353 \pm 76	530 \pm 61	8802 \pm 479	15%
5 β -Stigmastanol	58 \pm 5	nd	334 \pm 45	183 \pm 33	nd	20%
Epi-5β-stanols ($\mu\text{g g}^{-1}$)						
Epicoprostanol	1 \pm 1	62 \pm 14	25 \pm 8	88 \pm 30	1427 \pm 151	2.5%
Epi- 5β -stigmastanol	0	nd	0 \pm 0	nd	nd	3%
5α-Stanols ($\mu\text{g g}^{-1}$)						
5 α -Cholestanol	12 \pm 4	287 \pm 445	45 \pm 13	63 \pm 20	1668 \pm 199	8.5%
5 α -Stigmastanol	92 \pm 10	4685 \pm 617	127 \pm 17	nd	14329 \pm 658	10%
Stanones ($\mu\text{g g}^{-1}$)						
Coprostanone	3 \pm 2	nd	11 \pm 4	nd	nd	nd
Cholestanone	nd	nd	nd	nd	nd	nd
Ratios						
No. I	0.52 \pm -	0.88 ✓	0.89 ✓	0.91 ✓	0.86 ✓	0.67 \pm -
No. II	0.39 \pm -	-	0.72 ✓	-	-	0.70 \pm -
No. III	0.50 \pm -	0.87 ✓	0.89 ✓	0.89 ✓	0.84 ✓	0.64 \pm -
No. IV	-	-	-	-	-	-
No. V	17% ✓ (7-26%)	-	51% (42-60%)	74% (68-80%)	-	43%
No. VI	0.08 ✓ (0-0.4)	-	0.07 ✓ (0.04-0.12)	-	-	0.32 ✓

nd = not determined; [†] mean \pm standard deviation; [‡] mean \pm standard error

We only considered studies, in which steroid contents were presented and quantified (not considered: Bull et al., 1999; Evershed et al., 1997; Jardé et al., 2007; Standley et al., 2000)

Cited studies: 1: Leeming et al., 1996; 3: Shah et al., 2007 ($\mu\text{g g}^{-1}$ wet weight basis); 4: Tyagi et al., 2007; 7: Derrien et al., 2011 (only fresh faeces considered);

3: Results from Shah et al. (2007) presented here but excluded from further discussion due to extremely small 5 β -stigmastanol contents compared to all other studies

Diet of the studied animals: x = no information provided; c = wheat, soybean, rapeseed;

Ratios for a detection of faecal matter (and reference):

No. I: (coprostanol + epicoprostanol) / (5 α -cholestanol + coprostanol + epicoprostanol) (Bull et al., 1999);

No. II: (5 β -stigmastanol + epi-5 β -stigmastanol) / (5 α -stigmastanol + 5 β -stigmastanol + epi-5 β -stigmastanol)
(modified from Bull et al., 1999);

No. III: coprostanol / (5 α -cholestanol + coprostanol) (Grimalt et al., 1990);

No. IV: coprostanone / (cholestanone + coprostanone) (Grimalt et al., 1990);

Threshold values (Ratios No. I-IV):

>0.7 faecal input confirmed ✓; 0.3-0.7 faecal input can neither be confirmed nor excluded +/-; <0.3 faecal input should be excluded ✗

Ratios for a source identification of faecal matter:

No. V: coprostanol / (coprostanol + 5 β -stigmastanol) \times 100% (Leeming et al., 1997)

No. VI: epi-5 β -stigmastanol / 5 β -stigmastanol + epicoprostanol / coprostanol

Threshold values (Ratios No. V-VIII):

No. V: < 38% faeces of herbivores; > 73% human faeces (Leeming et al., 1997)

No. VI: > 1.2 horse faeces; < 0.8 no horse faeces

✓ source identification was possible; ✗ source identification was not possible.

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S8 Table (continuation). Sterol, stanol, and stanone contents of omnivore faeces (data from literature)

Steroid (trivial name)	Human ^{1x} (n=6)	Human ^{3x} (n=7)	Human ^{8d} (n=18)	Human ^{8e} (n=22)	Human ^{8f} (n=18)	Human ^{9g} (n=6)	Human ^{9h} (n=6)
Δ^5-Sterols ($\mu\text{g g}^{-1}$)							
Cholesterol	290 \pm 26 ^f	1201 \pm 574 ^f	nd	nd	nd	79 \pm 49 ^t	135 \pm 165 ^t
Stigmastanol	18 \pm 7	6 \pm 3	nd	nd	nd	nd	nd
β -Sitosterol	121 \pm 15	117 \pm 103	nd	nd	nd	13 \pm 13	70 \pm 77
5β-Stanols ($\mu\text{g g}^{-1}$)							
Coprostanol	3432 \pm 636	2036 \pm 577	20600	7400	9300	420 \pm 138	417 \pm 164
5 β -Stigmastanol	1245 \pm 263	15 \pm 4	nd	nd	nd	64 \pm 14	205 \pm 93
Epi-5β-stanols ($\mu\text{g g}^{-1}$)							
Epicoprostanol	52 \pm 19	0.03 \pm 0.02	nd	nd	nd	nd	nd
Epi- 5β -stigmastanol	0 \pm 0	nd	nd	nd	nd	nd	nd
5α-Stanols ($\mu\text{g g}^{-1}$)							
5 α -Cholestanol	70 \pm 15	62 \pm 38	nd	nd	nd	nd	nd
5 α -Stigmastanol	60 \pm 4	nd	nd	nd	nd	nd	nd
Stanones ($\mu\text{g g}^{-1}$)							
Coprostanone	29 \pm 6	nd	nd	nd	nd	27 \pm 10	63 \pm 32
Cholestanone	nd	nd	nd	nd	nd	nd	nd
Ratio							
No. I	0.98 ✓	0.97 ✓	-	-	-	-	-
No. II	0.95 ✓	-	-	-	-	-	-
No. III	0.98 ✓	0.97 ✓	-	-	-	-	-
No. IV	-	-	-	-	-	-	-
No. V	73% ✓ (65-81%)	99% ✓ (99-10)	-	-	-	87% ✓ (78-92)	67% ✗ (46-84)
No. VI	0.02 ✓ (0.01-0.03)	-	-	-	-	-	-

nd = not determined; ^t mean \pm standard deviation; ^f mean \pm standard error

We only considered studies, in which steroid contents were presented and quantified (not considered: Bull et al., 1999; Evershed et al., 1997; Jardé et al., 2007; Standley et al., 2000)

Cited studies: 1: Leeming et al., 1996; 3: Shah et al., 2007 ($\mu\text{g g}^{-1}$ wet weight basis); 8: Reddy et al., 1998 (only women); 9: Eneroeth et al., 1964 (only men)

3: Results from Shah et al. (2007) presented here but excluded from further discussion due to extremely small 5 β -stigmastanol contents compared to all other studies

Diet of the studied humans: x = no information provided; d = Caucasian omnivores; e = Indian vegetarians; f = Caucasian vegetarians; g = dietary fat is butter; h = dietary fat is corn oil

Ratios for a detection of faecal matter (and reference):

No. I: (coprostanol + epicoprostanol) / (5 α -cholestanol + coprostanol + epicoprostanol) (Bull et al., 1999);

No. II: (5 β -stigmastanol + epi-5 β -stigmastanol) / (5 α -stigmastanol + 5 β -stigmastanol + epi-5 β -stigmastanol) (modified from Bull et al., 1999);

No. III: coprostanol / (5 α -cholestanol + coprostanol) (Grimalt et al., 1990);

No. IV: coprostanone / (cholestanone + coprostanone) (Grimalt et al., 1990):

Threshold values (Ratios No. I-IV):

>0.7 faecal input confirmed ✓; 0.3-0.7 faecal input can neither be confirmed nor excluded +/-; <0.3 faecal input should be excluded ✗

Ratios for a source identification of faecal matter:

No. V: coprostanol / (coprostanol + 5 β -stigmastanol) x 100% (Leeming et al., 1997)

No. VI: epi-5 β -stigmastanol / 5 β -stigmastanol + epicoprostanol / coprostanol

Threshold values (Ratios No. V-VIII):

No. V: < 38% faeces of herbivores; > 73% human faeces (Leeming et al., 1997)

No. VI: > 1.2 horse faeces; < 0.8 no horse faeces

✓ source identification was possible; ✗ source identification was not possible.