

SUPPLEMENTAL INFORMATION

Quantitative Profiling of Seven Steroids in Saliva using LC-MS/MS

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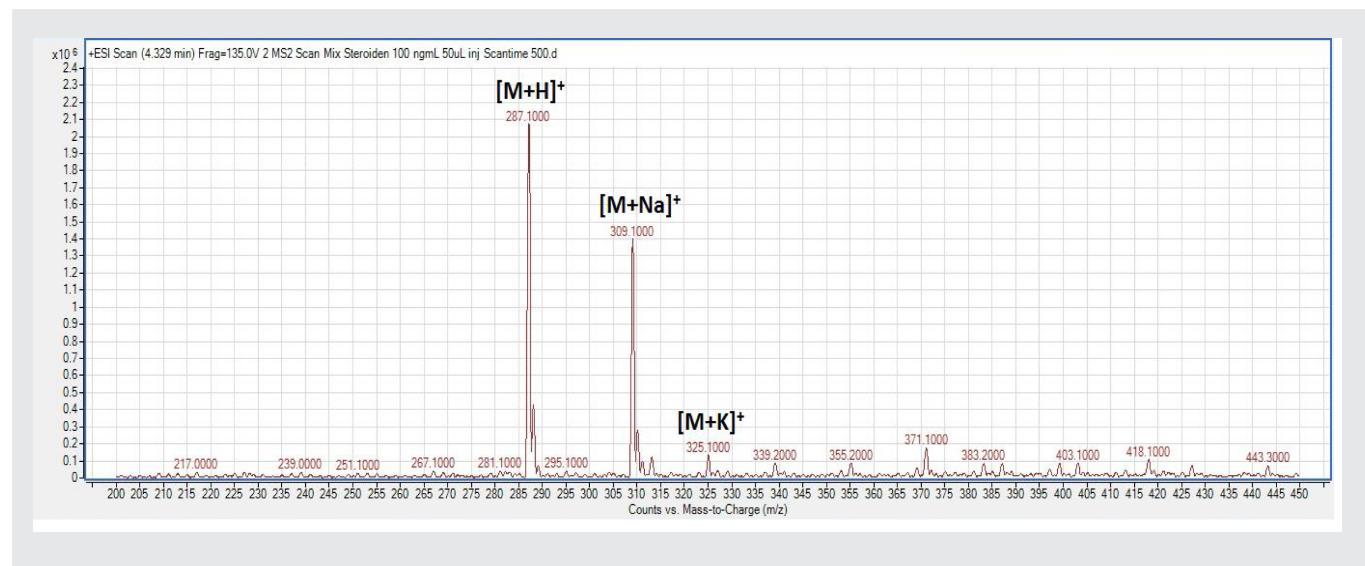


Figure S1. Full scan MS spectrum of a 100 ng/mL androstenedione solution in 50:50 methanol:water. The $[M+H]^+$ at 287.1 m/z, the $[M+Na]^+$ at 309.1 m/z and a small $[M+K]^+$ peak at 325.1 m/z are indicated.

Table S1. Observations for the investigated potential interferences.

Name	$[M+H]^+$ (m/z)	Retention time (min.)	Potentially interference tested for	Retention time difference
11 α -hydroxyprogesterone	331.2	-	17 α -hydroxyprogesterone	-
11 β -hydroxyprogesterone	331.2	10.50	17 α -hydroxyprogesterone	1.10
21-hydroxyprogesterone	331.2	10.16	17 α -hydroxyprogesterone	1.44
β -estradiol-6-one	287.2	-	Androstenedione	-
Aldosterone	361.2	4.94	Cortisone	0.86
Corticosterone	347.2	7.31	21-deoxycortisol	0.00
			11-deoxycortisol	0.29
Dehydroepiandrosterone	289.2	-	Testosterone	-
Epitestosterone	289.2	11.30	Testosterone	1.90
Estriol	289.2	-	Testosterone	-
Fenofibrate	361.8	-	Cortisone	-
Prednisolone	361.2	5.57	Cortisone	0.23

- = indicates that the analysis of that component did not result in a response in the current method.

Table S2a. Calibration function of the steroid cortisol.

Cortisol	a	b	R ²
Day 1	2.039	0.026	0.998
Day 2	1.954	0.029	0.999
Day 3	1.980	0.028	0.999
Day 4	1.894	0.024	1.000
Day 5	1.868	0.032	0.999
Average	1.947	0.028	0.999
Standard deviation	0.068	0.003	0.001

Table S2b. Calibration function of the steroid cortisone.

Cortisone	a	b	R ²
Day 1	4.790	-0.009	1.000
Day 2	4.800	-0.041	0.999
Day 3	4.922	-0.063	1.000
Day 4	4.840	-0.066	0.999
Day 5	4.810	-0.062	0.999
Average	4.832	-0.048	0.999
Standard deviation	0.053	0.024	0.000

Table S2c. Calibration function of the steroid 21-deoxycortisol.

21-deoxycortisol	a	b	R ²
Day 1	1.160	-0.001	0.999
Day 2	1.115	-0.003	0.999
Day 3	1.097	0.000	1.000
Day 4	1.108	0.000	1.000
Day 5	1.059	0.002	1.000
Average	1.108	0.000	0.999
Standard deviation	0.036	0.002	0.000

Table S2d. Calibration function of the steroid 11-deoxycortisol.

11-deoxycortisol	a	b	R ²
Day 1	2,040	-0,005	0,999
Day 2	1,996	-0,008	1,000
Day 3	1,979	-0,004	1,000
Day 4	1,942	0,001	1,000
Day 5	1,939	-0,004	1,000
Average	1,979	-0,004	1,000
Standard deviation	0,042	0,003	0,000

Table S2e. Calibration function of the steroid testosterone.

Testosterone	a	b	R²
Day 1	1.078	-0.002	0.999
Day 2	1.070	-0.002	1.000
Day 3	1.078	-0.001	1.000
Day 4	1.055	-0.001	1.000
Day 5	1.056	-0.001	0.999
Average	1.067	-0.001	1.000
Standard deviation	0.012	0.000	0.000

Table S2f. Calibration function of the steroid androstenedione.

Androstenedione	a	b	R²
Day 1	0.866	0.000	0.999
Day 2	0.859	-0.001	1.000
Day 3	0.864	0.000	1.000
Day 4	0.858	-0.001	1.000
Day 5	0.854	0.000	0.999
Average	0.860	0.000	1.000
Standard deviation	0.005	0.000	0.000

Table S2g. Calibration function of the steroid 17 α OHP.

17αOHP	a	b	R²
Day 1	0.952	-0.004	0.999
Day 2	0.914	-0.001	1.000
Day 3	0.924	0.000	1.000
Day 4	0.906	-0.002	0.999
Day 5	0.913	-0.001	0.999
Average	0.922	-0.002	0.999
Standard deviation	0.018	0.001	0.000