SUPPORTING INFORMATION

INTERLABORATORY AND INTERPLATFORM STUDY OF STEROIDS COLLISION CROSS SECTION BY TRAVELING WAVE ION MOBILITY SPECTROMETRY

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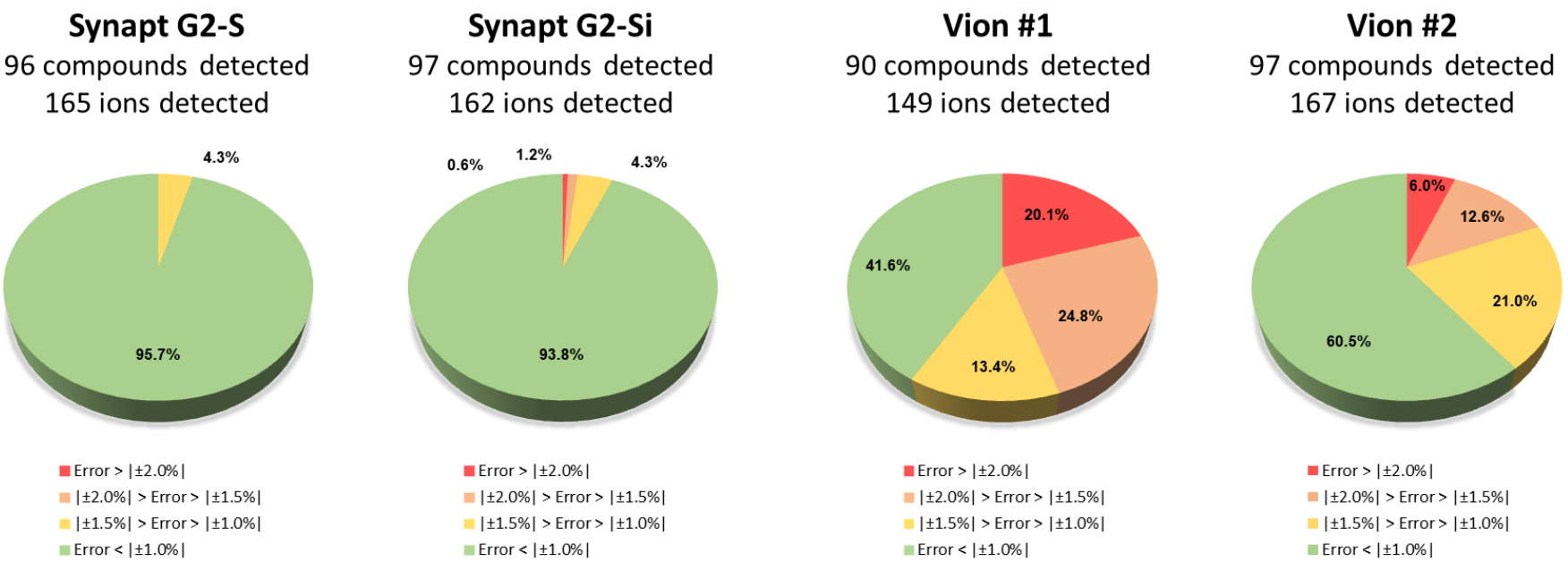

Figure S1. Bias observed between $^{TW}CCS_{N_2}$ measurements and database values[1,2] for a total number of 97 steroids involving 167 ions. The number of compounds and ions detected by each TWIMS-TOF-MS instrument is indicated above each graph.

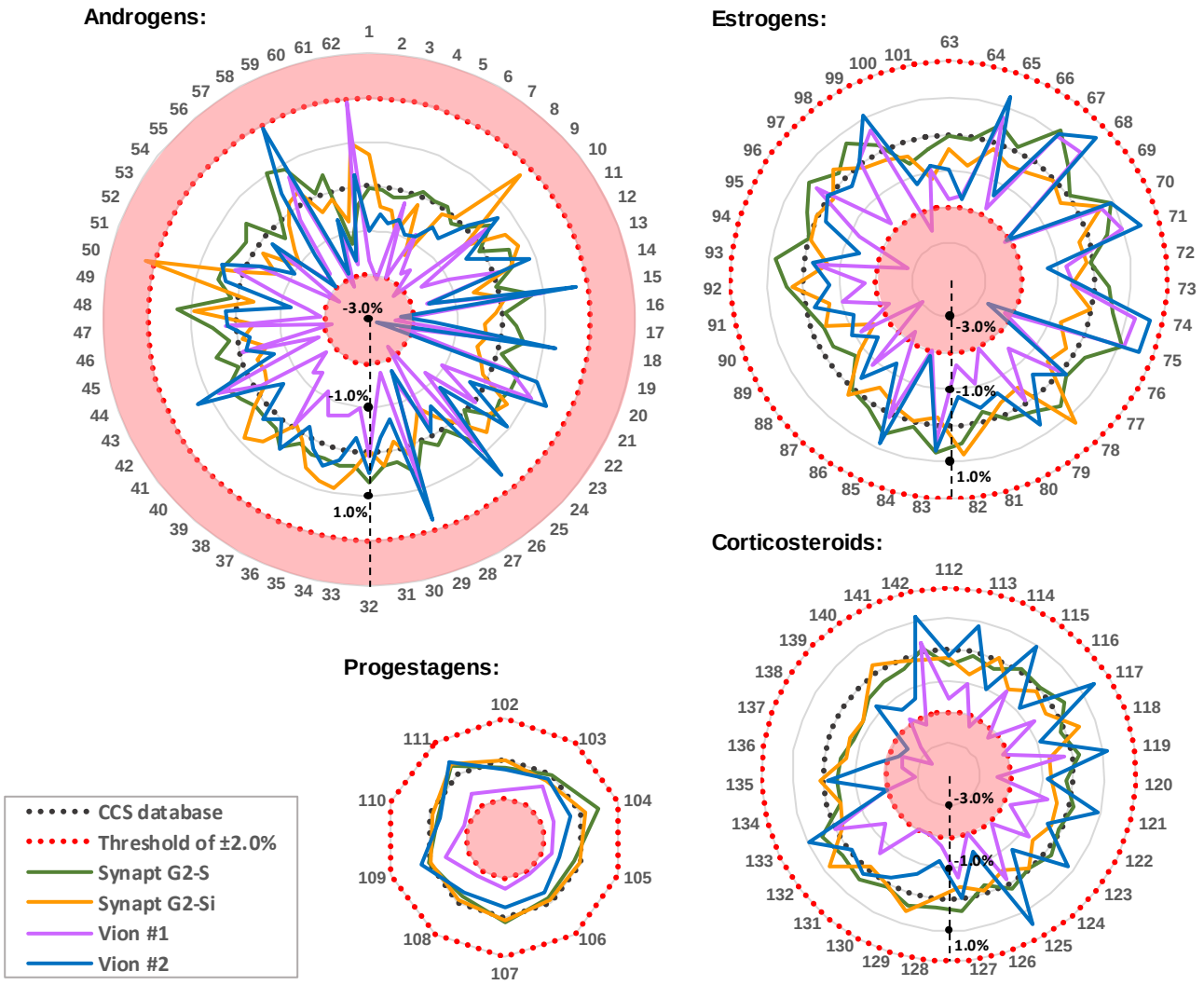

Figure S2. Deviations existing between the $^{TW}CCS_{N_2}$ values measured by the four TWIMS instruments and the values previously reported by databases[1,2]. Red zones indicate a bias greater than ±2%, whereas the dashed black line indicates that not bias (0%) from the CCS database was observed. Only those ions detected by all instruments were included in this graph (n = 142). See Table S1 for compounds identification.

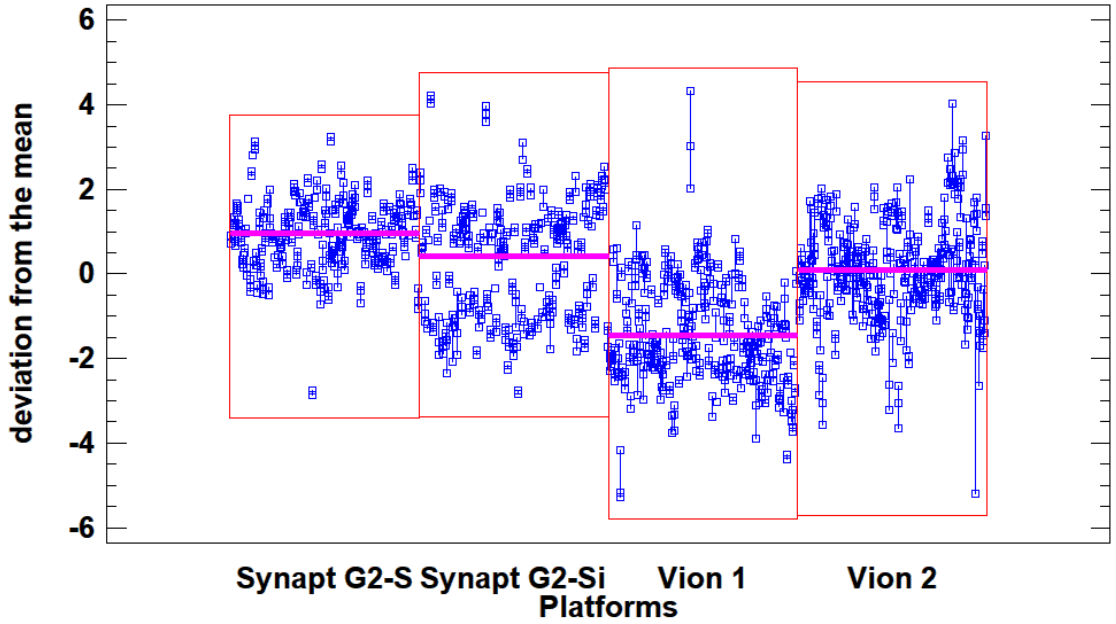

Figure S3. Deviations (in $Å^2$) between $^{TW}CCS_{N_2}$ measurements (in triplicate) performed by each TWIMS instrument and average values (i.e. cross-laboratory database). The global deviation of each instrument (in $Å^2$) is indicated by the pink lines.

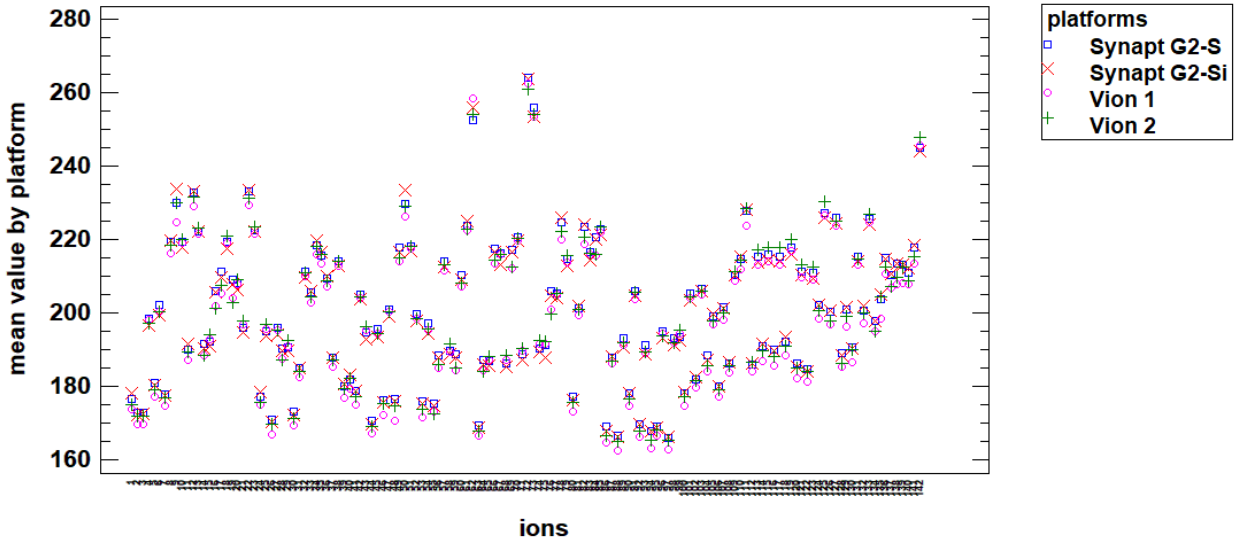

Figure S4. Representation of the $^{TW}CCS_{N_2}$ values (Å^2) measured for each ion (n = 142) by the four TWIMS instruments. A number has been assigned to each ion according to Table S1.

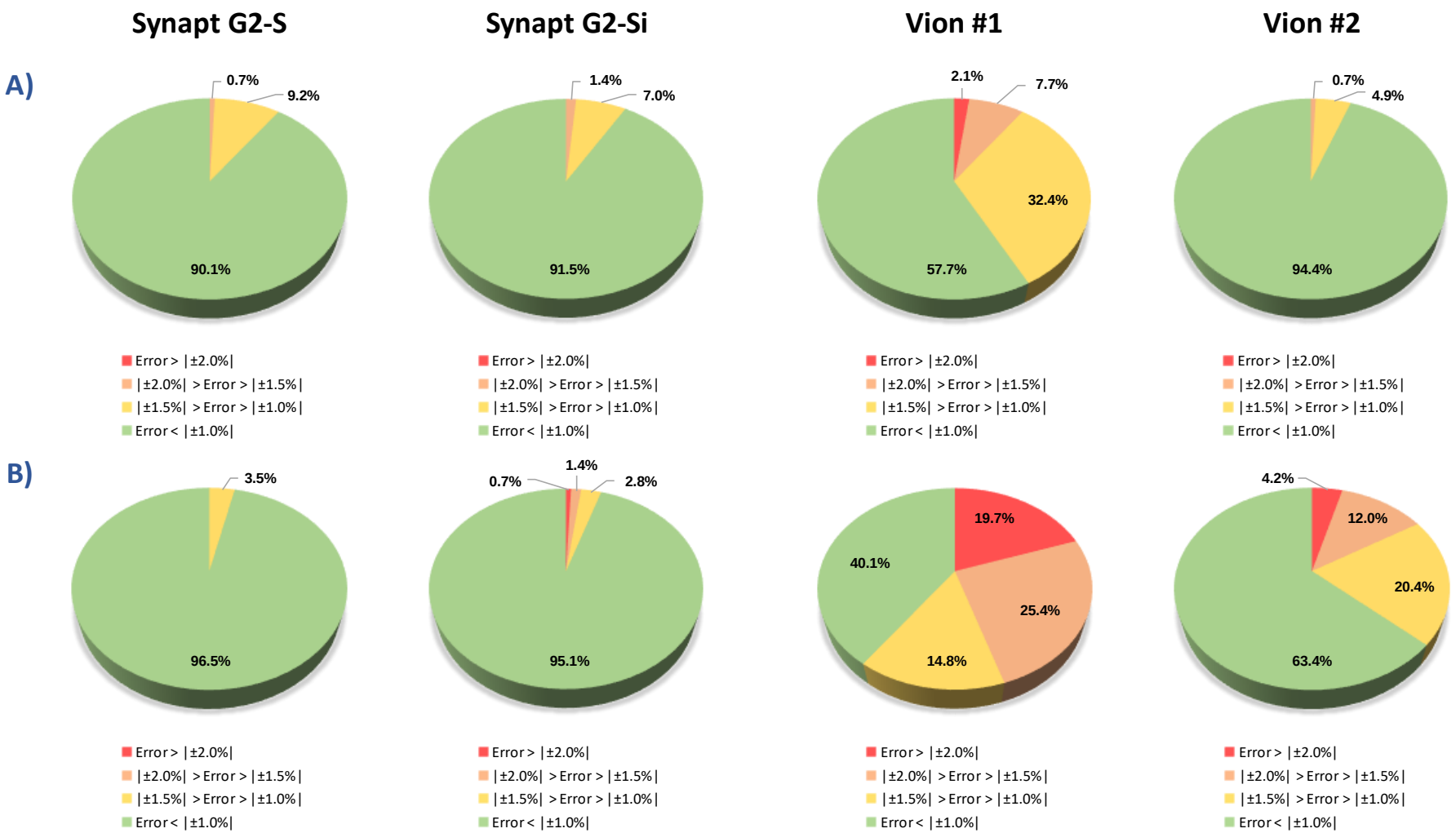

Figure S5. Bias observed between $^{TW}CCS_{N_2}$ measurements performed by each TWIMS instrument and: A) average $^{TW}CCS_{N_2}$ values (resulted from their measurement in triplicate by four TWIMS instrument), B) the initial (i.e. single-laboratory) database values.[1,2] In total, 87 steroids involving 142 ions were investigated.

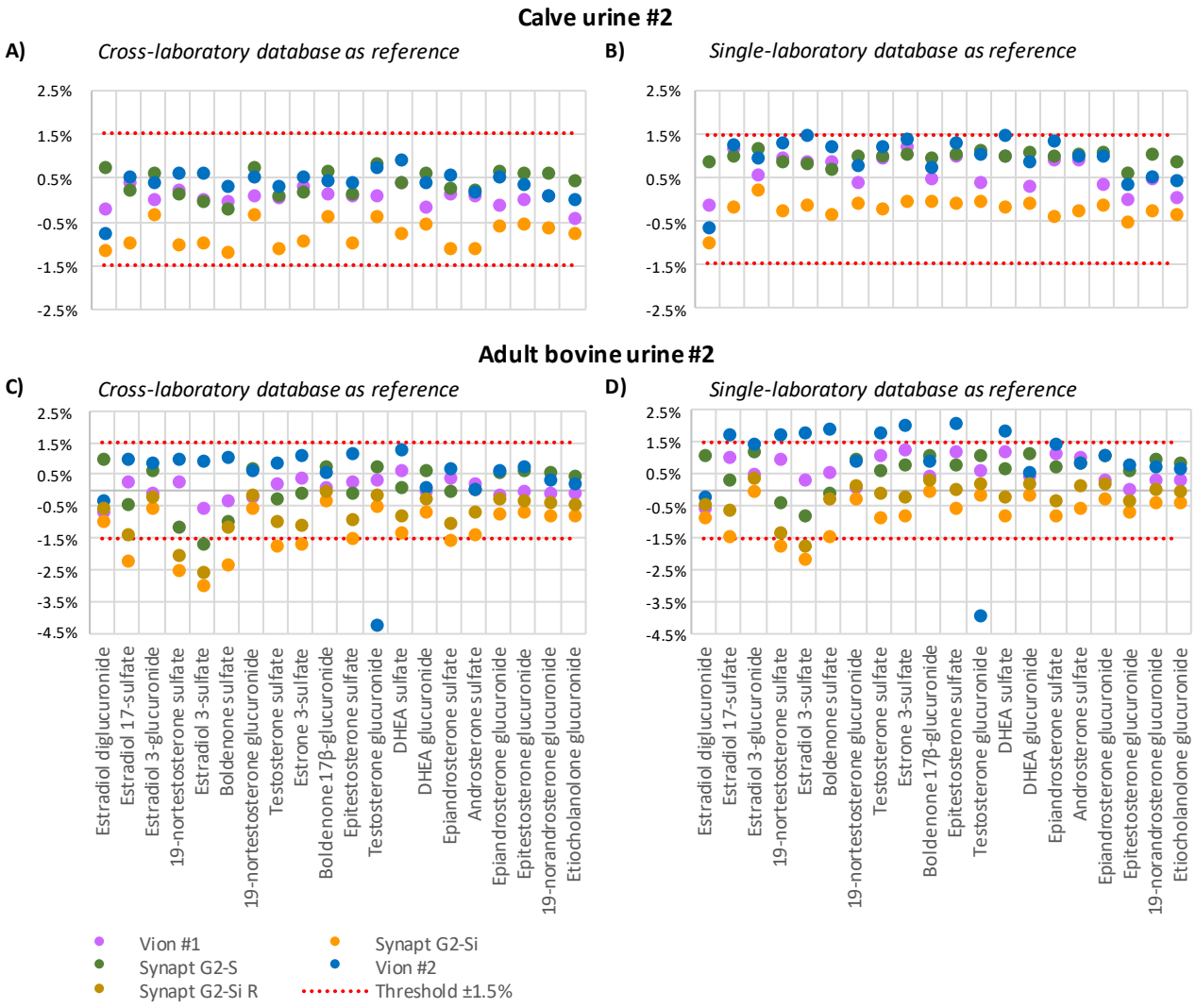

Figure S6. Bias between $^{TW}CCS_{N_2}$ measurements in each TWIMS instrument and (A and C) the cross-laboratory database or (B and D) the single-laboratory database. Phase II steroid metabolites in calve and adult bovine urine samples were investigated. $^{TW}CCS_{N_2}$ measurements are related to the $[M-H]^-$ ion of each molecule and were performed in triplicate by each instrument.

Table S1. Identification number of each ionized steroid and related to Figure S2.

ID	Compound and ion	ID	Compound and ion	ID	Compound and ion
1	androstanedione; $[M+H]^+$	49	boldenone glucuronide; $[M+H]^+$	97	trenbolone; $[M+H]^+$
2	testosterone; $[M+H]^+$	50	boldenone glucuronide; $[M+Na]^+$	98	trenbolone; $[M+Na]^+$
3	epitestosterone; $[M+H]^+$	51	boldenone glucuronide; $[M-H]^-$	99	estriol 3-sulfate; $[M-H]^-$
4	epitestosterone; $[M+Na]^+$	52	oral turinabol; $[M+Na]^+$	100	gestrinone; $[M+H]^+$
5	methyl-chlorotestosterone; $[M+H]^+$	53	4-chlorotestosterone; $[M+H]^+$	101	gestrinone; $[M+Na]^+$
6	methyl-chlorotestosterone; $[M+Na]^+$	54	4-chlorotestosterone; $[M+Na]^+$	102	17-hydroxyprogesterone; $[M+H]^+$
7	methyltestosterone; $[M+H]^+$	55	16α-hydroxytestosterone; $[M+H]^+$	103	17-hydroxyprogesterone; $[M+Na]^+$
8	testosterone glucuronide; $[M+H]^+$	56	boldenone sulfate; $[M+H]^+$	104	danazol; $[M+H]^+$
9	testosterone glucuronide; $[M+Na]^+$	57	boldenone sulfate; $[M+Na]^+$	105	medroxyprogesterone acetate; $[M+H]^+$
10	testosterone glucuronide; $[M-H]^-$	58	boldenone sulfate; $[M-H]^-$	106	progesterone; $[M+H]^+$
11	stanozolol; $[M+H]^+$	59	4-chlorotestosterone acetate; $[M+H]^+$	107	melengestrol acetate; $[M+H]^+$
12	DHEA glucuronide; $[M+Na]^+$	60	4-chlorotestosterone acetate; $[M+Na]^+$	108	medroxyprogesterone; $[M+H]^+$
13	DHEA glucuronide; $[M-H]^-$	61	boldenone undecylenate; $[M+H]^+$	109	medroxyprogesterone; $[M+Na]^+$
14	epitestosterone sulfate; $[M+H]^+$	62	boldenone undecylenate; $[M+Na]^+$	110	17-caproxyprogesterone; $[M+H]^+$
15	epitestosterone sulfate; $[M-H]^-$	63	19-nortestosterone; $[M+H]^+$	111	17-caproxyprogesterone; $[M+Na]^+$
16	epitestosterone glucuronide; $[M+H]^+$	64	19-nortestosterone sulfate; $[M+H]^+$	112	cortisone; $[M+H]^+$
17	epitestosterone glucuronide; $[M+Na]^+$	65	19-nortestosterone sulfate; $[M-H]^-$	113	betamethasone; $[M+Na]^+$
18	epitestosterone glucuronide; $[M-H]^-$	66	19-nortestosterone glucuronide; $[M+H]^+$	114	dexamethasone; $[M+H]^+$
19	etiocholanolone glucuronide; $[M+Na]^+$	67	19-nortestosterone glucuronide; $[M-H]^-$	115	dexamethasone; $[M+Na]^+$
20	etiocholanolone glucuronide; $[M-H]^-$	68	estradiol 17-sulfate; $[M-H]^-$	116	triamcinolone; $[M+H]^+$
21	epiandrosterone sulfate; $[M-H]^-$	39	estradiol 3-glucuronide; $[M+Na]^+$	117	triamcinolone; $[M+Na]^+$
22	epiandrosterone glucuronide; $[M+Na]^+$	70	estradiol 3-glucuronide; $[M-H]^-$	118	flumethasone; $[M+H]^+$
23	epiandrosterone glucuronide; $[M-H]^-$	71	estrone 3-sulfate; $[M-H]^-$	119	flumethasone; $[M+Na]^+$
24	stanolone; $[M+H]^+$	72	estradiol diglucuronide; $[M+Na]^+$	120	prednisolone; $[M+H]^+$
25	androsterone sulfate; $[M-H]^-$	73	estradiol diglucuronide; $[M-H]^-$	121	prednisolone; $[M+Na]^+$
26	boldenone; $[M+H]^+$	74	estradiol 3-sulfate; $[M-H]^-$	122	prednisone; $[M+H]^+$
27	boldenone; $[M+Na]^+$	75	17α-estradiol 3-sulfate; $[M-H]^-$	123	prednisone; $[M+Na]^+$
28	testosterone sulfate; $[M+H]^+$	76	19-noretiocholanolone glucuronide; $[M+Na]^+$	124	flunisolide; $[M+H]^+$
29	testosterone sulfate; [M-H]-	77	19-noretiocholanolone glucuronide; $[M-H]^-$	125	flunisolide; $[M+Na]^+$
30	androstenedione; $[M+H]^+$	78	19-norandrosterone glucuronide; $[M+Na]^+$	126	desonide; $[M+H]^+$
31	testosterone acetate; [M+H]+	79	19-norandrosterone glucuronide; $[M-H]^-$	127	desonide; $[M+Na]^+$
32	testosterone acetate; $[M+Na]^+$	80	norethindrone; $[M+H]^+$	128	18-hydroxycortisol; $[M+H]^+$
33	testosterone benzoate; $[M+H]^+$	81	19-nortestosterone benzoate; $[M+H]^+$	129	18-hydroxycortisol; $[M+Na]^+$
34	testosterone cypionate; $[M+H]^+$	82	estradiol 17-glucuronide; $[M+Na]^+$	130	6α-methylprednisolone; $[M+H]^+$
35	testosterone enanthate; $[M+H]^+$	83	estradiol 17-glucuronide; $[M-H]^-$	131	6α-methylprednisolone; $[M+Na]^+$
36	testosterone 4-methylvalerate; $[M+H]^+$	84	estriol 3-glucuronide; $[M+Na]^+$	132	triamcinolone acetonide; $[M+H]^+$
37	boldenone propionate; $[M+H]^+$	85	estriol 3-glucuronide; $[M-H]^-$	133	triamcinolone acetonide; $[M+Na]^+$
38	boldenone propionate; $[M+Na]^+$	86	16α-hydroxyestrone; $[M+H]^+$	134	cortisol 21-acetate; $[M+H]^+$
39	mesterolone; $[M+H]^+$	87	norethindrone acetate; $[M+H]^+$	135	cortisol 21-acetate; $[M+Na]^+$
40	mestanolone; $[M+H]^+$	88	epitrenbolone; $[M+H]^+$	136	hydrocortisone hemisuccinate; $[M+H]^+$
41	fluoxymesterone; $[M+H]^+$	89	epitrenbolone; $[M+Na]^+$	137	hydrocortisone hemisuccinate; $[M+Na]^+$
42	fluoxymesterone; $[M+Na]^+$	90	trenbolone acetate; $[M+H]^+$	138	prednisolone 21-hemisuccinate; $[M+H]^+$
43	DHEA sulfate; $[M-H]^-$	91	trenbolone acetate; $[M+Na]^+$	139	prednisolone 21-hemisuccinate; $[M+Na]^+$
44	boldione; $[M+H]^+$	92	4-fluoro-19-nortestosterone; $[M+H]^+$	140	triamcinolone 16,21-diacetate; $[M+H]^+$
45	boldione; $[M+Na]^+$	93	4-fluoro-19-nortestosterone; $[M+Na]^+$	141	triamcinolone 16,21-diacetate; $[M+Na]^+$
46	dianabol; $[M+H]^+$	94	11-ketoestrone; $[M+H]^+$	142	diflucortolone pivalate; $[M+Na]^+$
47	dianabol; $[M+Na]^+$	95	epi-19-nortestosterone; $[M+H]^+$		
48	14α-hydroxytestosterone; $[M+H]^+$	96	epi-19-nortestosterone; $[M+Na]^+$		

REFERENCES

[1] Hernández-Mesa, M.; Le Bizec, B.; Monteau, F.; García-Campaña, A.M.; Dervilly-Pinel, G. *Anal. Chem.* **2018**, 90, 4616-4625.

[2] Hernández-Mesa, M.; Monteau, F.; Le Bizec, B.; Dervilly-Pinel, G. *Anal. Chim. Acta: X*, **2019**, 100006.