Electronic Supplementary Material (ESI) for Analytical Methods.
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Versatile UHPLC-MSMS method for simultaneous quantification of various alcohol intake related compounds in human urine and blood

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Supporting Information:

Table S–1. Table overview of LC gradient.

Time (min.)	Flow (mL min^{-1})	A:B	Curve
0	0.55	98:2	6
1	0.55	98:2	6
1.5	0.43	75:25	6
1.9	0.43	50:50	6
4.1	0.6	20:80	6
4.5	0.6	0:100	3
4.9	0.6	0:100	6
5.1	0.55	98:2	3
6	0.55	98:2	6

Table S–2. Overview of mass spectrometry parameters of target compounds with related internal standards (span = ±0.2; dwell = 0.100 s).

Compound	**RT**	**RT window**	**Primary transition** (quantifier)	**Secondary transition** (qualifier)	**Cone voltage**	**Collision E**
L– (+)–tartaric acid	0.56	0–0.85	149.1→87.1	149.1→73	25	[a]10 / [b]15
L– (+)–tartaric acid–d_2	0.55	0–0.85	151.1→74	151.1→88.1	25	15
ethyl sulphate	0.80	0.65–1.15	125→97	125→80	25	20
ethyl sulphate–d_5	0.79	0.65–1.15	130→98	130→80	25	20
ethyl-β-D-glucuronide	1.39	1–1.65	221.2→85.1	221.2→75.1	25	15
ethyl-β-D-glucuronide–d_5	1.34	1–1.65	226.2→85.1	226.2→75.1	25	15
indoxyl sulphate	2.54	2.35–2.75	212→80	212→132	30	20
indoxyl sulphate–d_4	2.53	2.35–2.75	216→80	216→136	30	20
p–cresol sulphate	2.68	2.65–3	186.7→107	186.7→80	30	20
p–cresol sulphate–d_7	2.80	2.25–2.8	194.1→114.1	194.1→80	30	20
resveratrol	[c]3.04/ 3.26	2.85–3.55	227.1→143.2	227.1→185	30	[a]25 / [b]20
resveratrol–$^{13}C_6$	[c]3.04/ 3.25	2.85–3.55	233.2→149.2	233.2→191.2	35	[a]25 / [b]20
estrone 3–sulphate	3.75	3.6–4	349.2→269.4	349.2→80	35	30
estrone–d_4– 3–sulphate	3.76	3.6–4	353.2→273.4	353.2→80	35	30
DHEAS	4.12	3.9–4.45	367.2→97	–	30	30
DHEAS–d_5	4.13	3.9–4.45	372.2→98	–	30	30

RT – retention time; [a]value for primary transition; [b]value for secondary transition; [c]commercial resveratrol is a mixture of *cis*– and *trans*–resveratrol

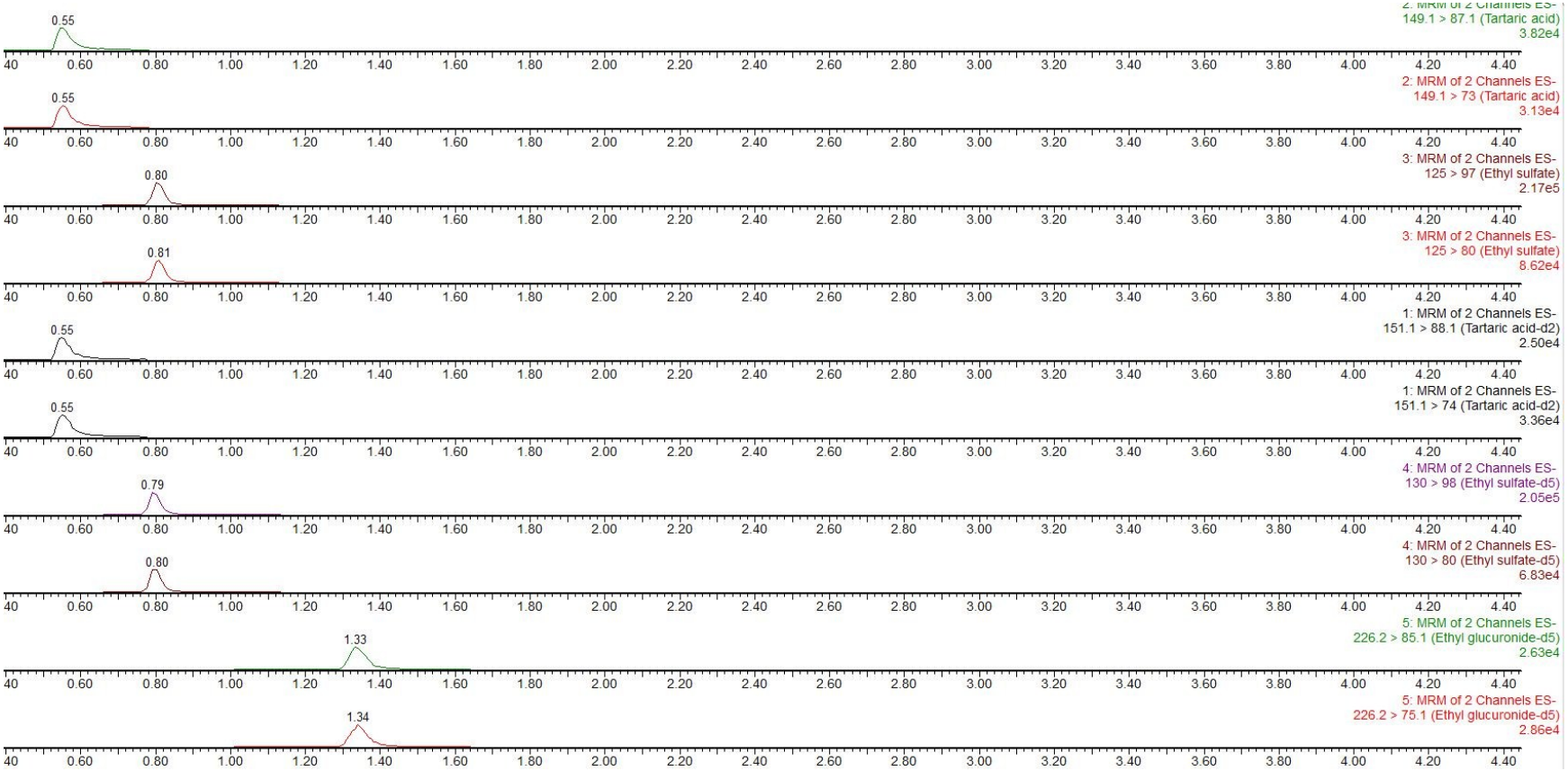
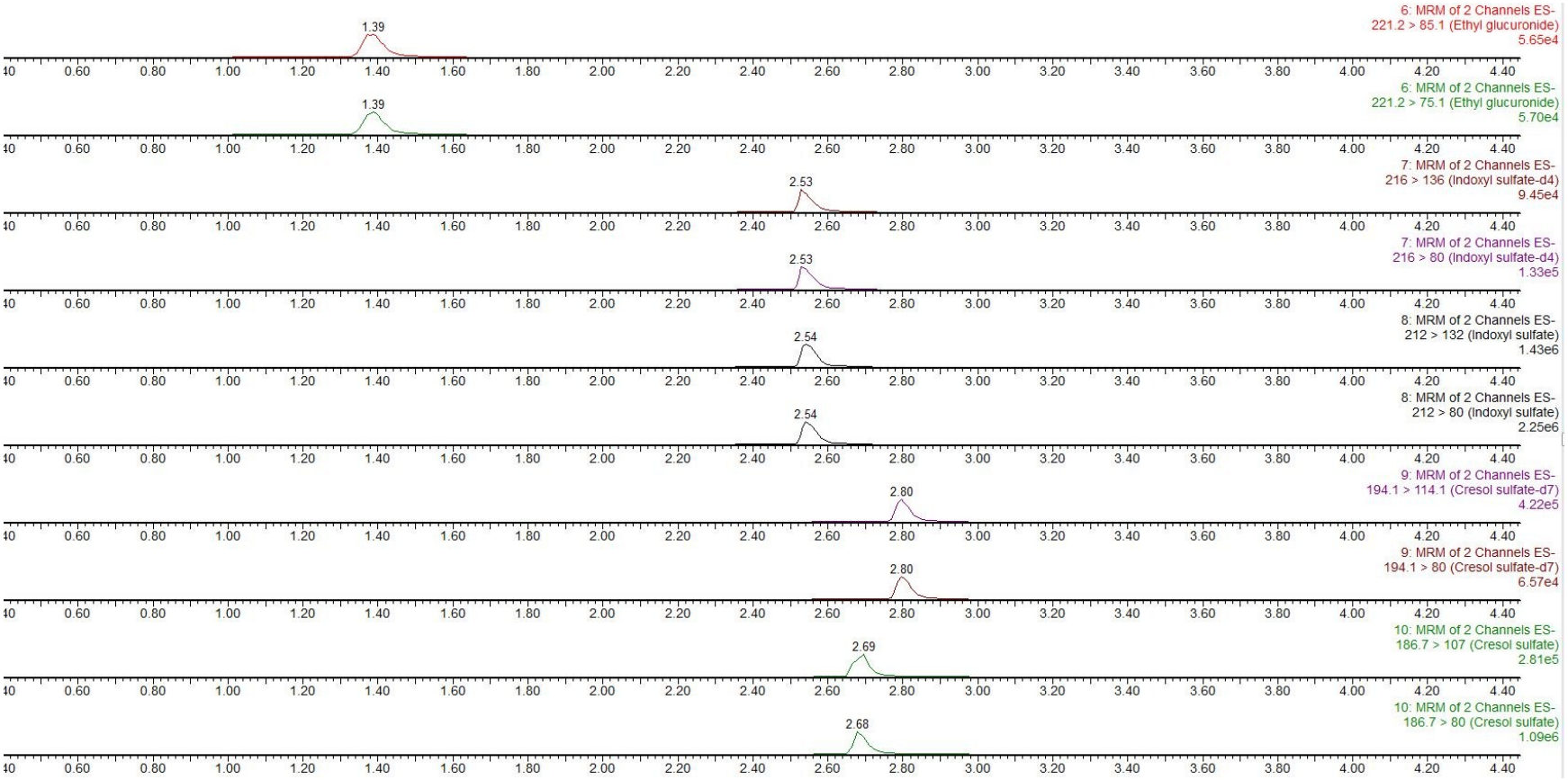


Figure S-1. Illustrative chromatograms of target compounds and related internal standards.



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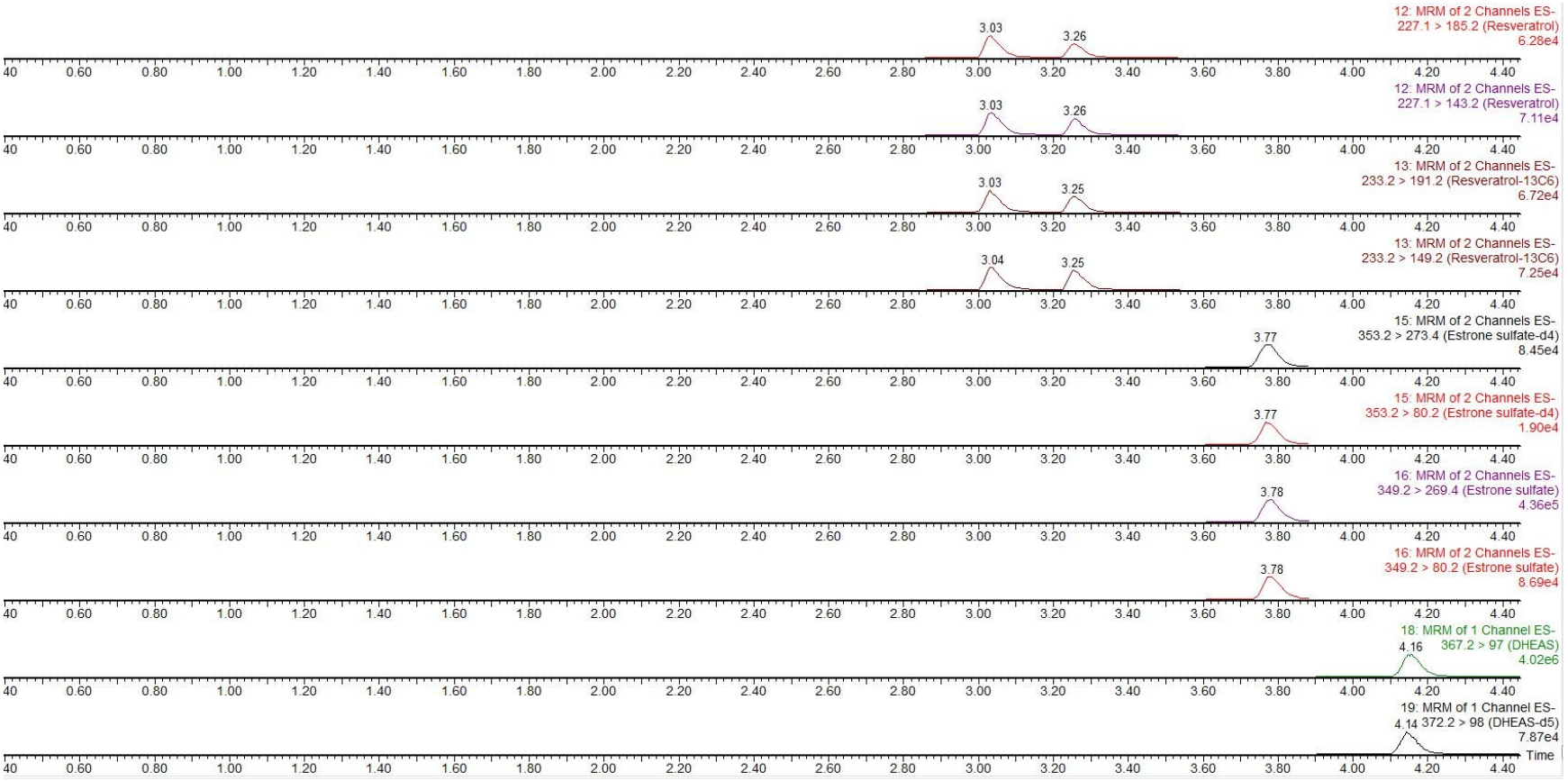

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Table S–3. Coefficients of variation (%) of repeatability (n=6) and intermediate precision (n=9).

Analyte	Repeatability			Intermediate precision		
	Standard solution	Urine	Plasma	Standard solution	Urine	Plasma
L-(+)-tartaric acid	1.7	1.4	2.0	3.5	2.0	3.3
ethyl sulphate	8.7	1.7	11	12	8.2	26
ethyl-β-D-glucuronide	3.3	1.6	2.1	3.9	3.2	2.5
indoxyl sulphate	2.5	2.1	2.7	3.4	1.8	1.9
***p*-cresol sulphate**	4.2	2.1	3.8	4.5	2.3	19
resveratrol	2.1	1.7	1.6	7.5	3.3	3.7
estrone 3-sulphate	1.5	1.8	1.1	2.5	2.0	4.5
DHEAS	0.51	0.97	1.1	0.90	1.3	1.7

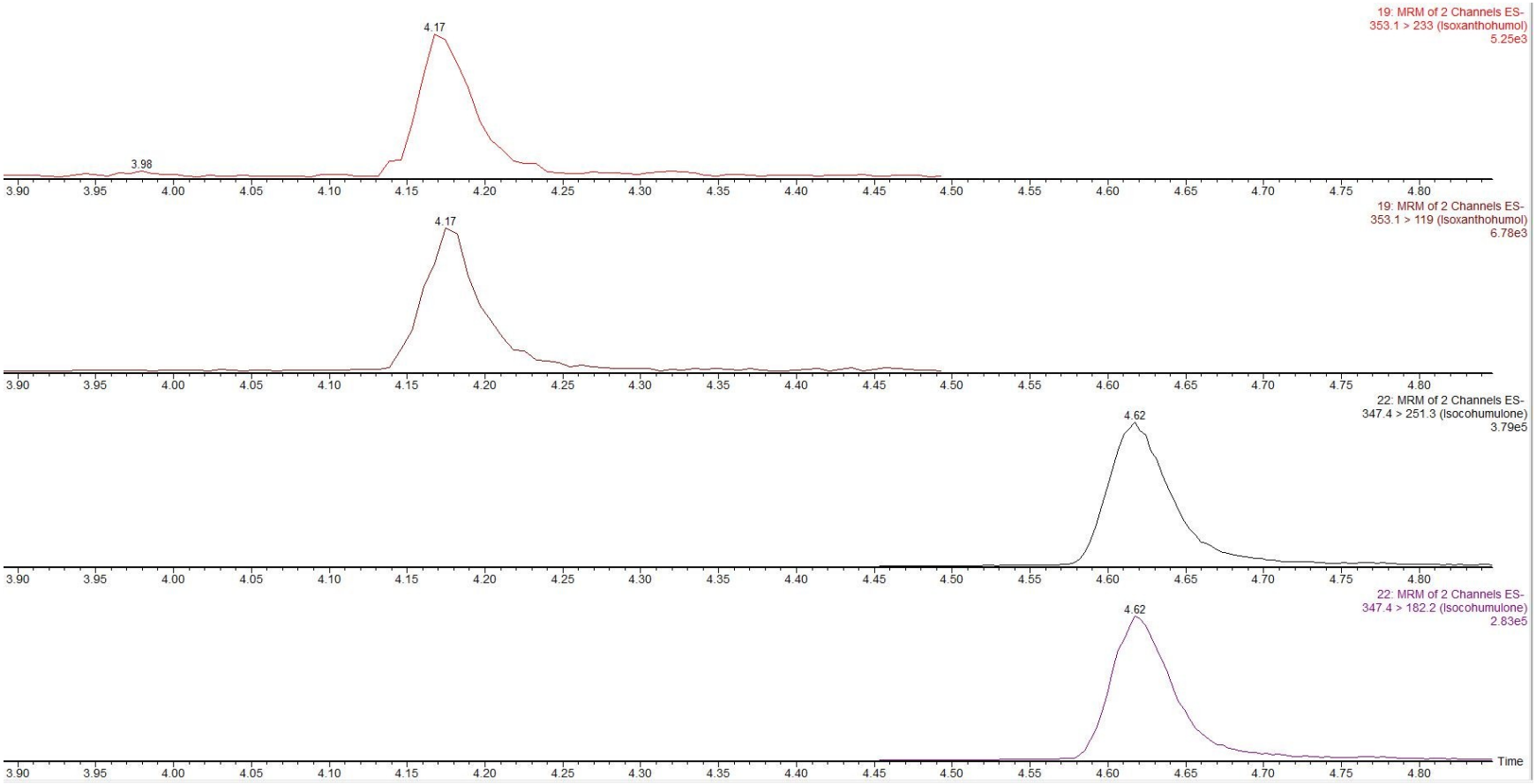

Figure S–2a. Illustrative chromatograms of isoxanthohumol and isocohumulone in 10× diluted pilsner beer.

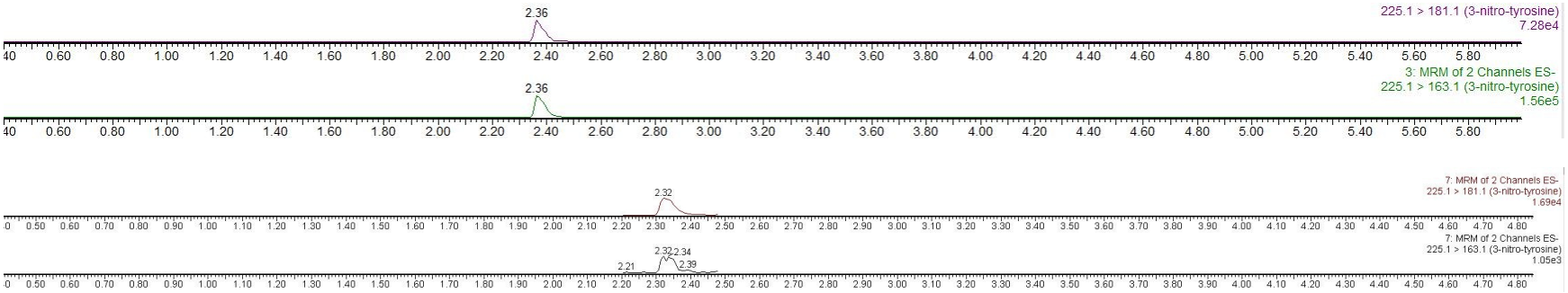

Figure S–2b. Illustrative chromatograms of 3–nitro–tyrosine in a standard solution (1 µg mL^{-1}) and an unknown isomer in pooled sample (n=80).

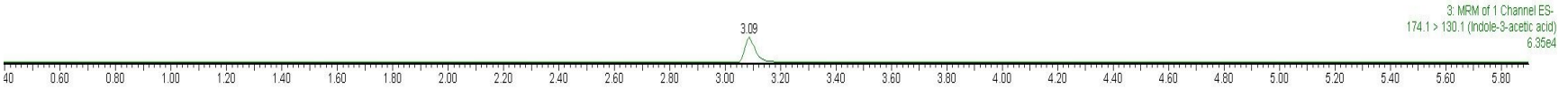

Figure S–2c. Illustrative chromatogram of indole–3–acetic acid in a standard solution.

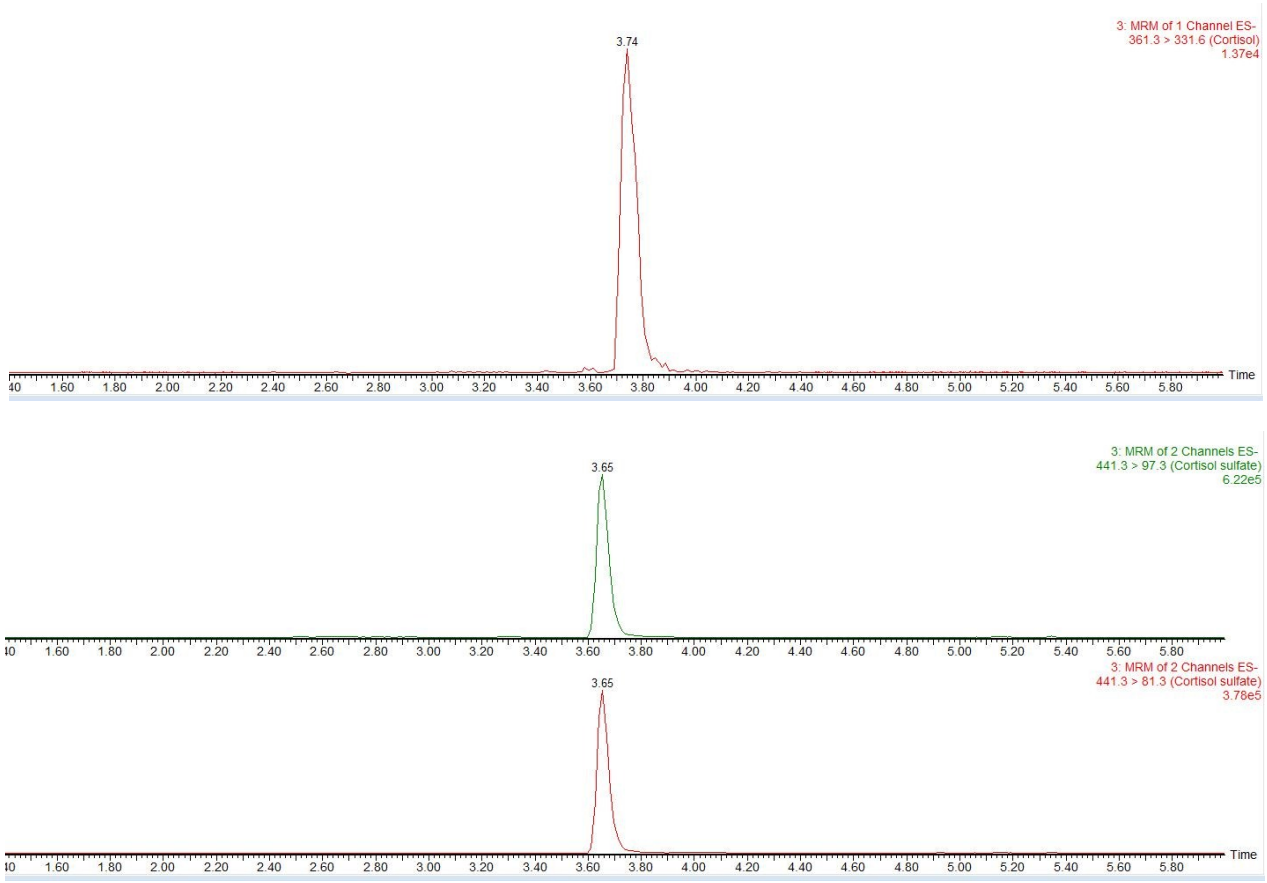

Figure S–2d. Illustrative chromatograms of cortisol and cortisol sulphate in standard solution.