Electronic Supplementary Material (ESI) for Analytical Methods.

Determination of sedative-hypnotics in human hair by micropulverized extraction and liquid chromatography/quadrupole-Orbitrap mass spectrometry.

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Supplementary Information (SI)

Content:

Table S1 Acquisition and calibration parameters

Analytes and internal standards	Molecular formula	Monoisotopic mass of protonated molecule	Time range (min)	Calibration parameters					
				Internal standard	Curve index	Weighting	Origin	Equation (y: peak area; x: concentration in pg mg^{-1})	R^2
alprazolam (ALP)	$C_{17}H_{13}ClN_4$	309.090	22.0-24.5	ALP-d_5	Linear	$1/x^2$	Ignore	y = -0.00129741 + 0.00255162x	0.9925
brotizolam (BROT)	$C_{15}H_{10}BrClN_4S$	392.957	27.0-30.0	TRI-d_4	Linear	$1/x^2$	Ignore	y = -0.000356934 + 0.00097534x	0.9905
N-desmethyldiazepam (DMD)	$C_{15}H_{11}ClN_2O$	271.063	24.0-26.5	DMD-d_5	Quadratic	Equal	Force	$y = 0.00336914x + 1.38188\times10^{-8}x^2$	0.9999
N-desmethylfludiazepam (DMF)	$C_{15}H_{10}ClFN_2O$	289.054	26.0-28.5	DMF-d_4	Linear	$1/x^2$	Ignore	y = -0.000924251 + 0.00286056x	0.9974
diazepam (DIA)	$C_{16}H_{13}ClN_2O$	285.079	30.0-35.0	DIA-d_5	Quadratic	Equal	Force	$y = 0.00290374x - 1.11029\times10^{-7}x^2$	0.9995
estazolam (EST)	$C_{16}H_{11}ClN_4$	295.075	15.0-23.0	EST-d_5	Linear	$1/x^2$	Ignore	y = 9.62685e-005 + 0.00274179x	0.9976
etizolam (ETI)	$C_{17}H_{15}ClN_4S$	343.078	27.0-30.0	TRI-d_4	Linear	$1/x^2$	Ignore	y = -0.000797923 + 0.00368474x	0.9893
flunitrazepam (FLUN)	$C_{16}H_{12}FN_3O_3$	314.094	27.0-30.0	FLUN-d_7	Linear	$1/x^2$	Ignore	y = 0.000178267 + 0.00276029x	0.9973
nitrazepam (NIT)	$C_{15}H_{11}N_3O_3$	282.087	15.0-23.0	NIT-d_5	Linear	$1/x^2$	Ignore	y = 0.000464354 + 0.00245904x	0.9892
ramelteon (RAM)	C16H21NO2	260.165	25.0-28.0	DMF-d_4	Linear	$1/x^2$	Ignore	y = 0.000804807 + 0.00385956x	0.9929
triazolam (TRI)	$C_{17}H_{12}Cl_2N_4$	343.051	23.0-26.5	TRI-d_4	Linear	$1/x^2$	Ignore	y = 0.000289182 + 0.00241819x	0.9871
zolpidem (ZOL)	$C_{19}H_{21}N_3O$	308.176	12.5-20.0	ZOL-d_6	Linear	$1/x^2$	Ignore	y = 0.00019509 + 0.00163075x	0.9972
zopiclone (ZOP)	$C_{17}H_{17}ClN_6O_3$	389.112	8.0-13.5	ZOP-d_4	Linear	$1/x^2$	Ignore	y = -0.00115316 + 0.0028835x	0.9967
ALP-d_5	$C_{17}H_8D_5ClN_4$	314.122	22.0-24.5						
DMD-d_5	$C_{15}H_6D_5ClN_2O$	276.095	24.0-26.5						
DMF-d_4	$C_{15}H_6D_4ClFN_2O$	293.079	26.0-28.5						
DIA-d_5	$C_{16}H_8D_5ClN_2O$	290.110	30.0-35.0						
EST-d_5	$C_{16}H_6D_5ClN_4$	300.106	15.0-23.0						
FLUN-d_7	$C_{16}H_5D_7FN_3O_3$	321.137	27.0-30.0						
NIT-d_5	$C_{15}H_6D_5N_3O_3$	287.119	15.0-23.0						
TRI-d_4	$C_{17}H_8D_4Cl_2N_4$	347.076	25.0-28.0						
ZOL-d_6	$C_{19}H_{16}D_6N_3O$	314.213	23.0-26.5						
ZOP-d_4	$C_{17}H_{13}D_4ClN_6O_3$	393.137	12.5-20.0						

R^2, Coefficient of determination

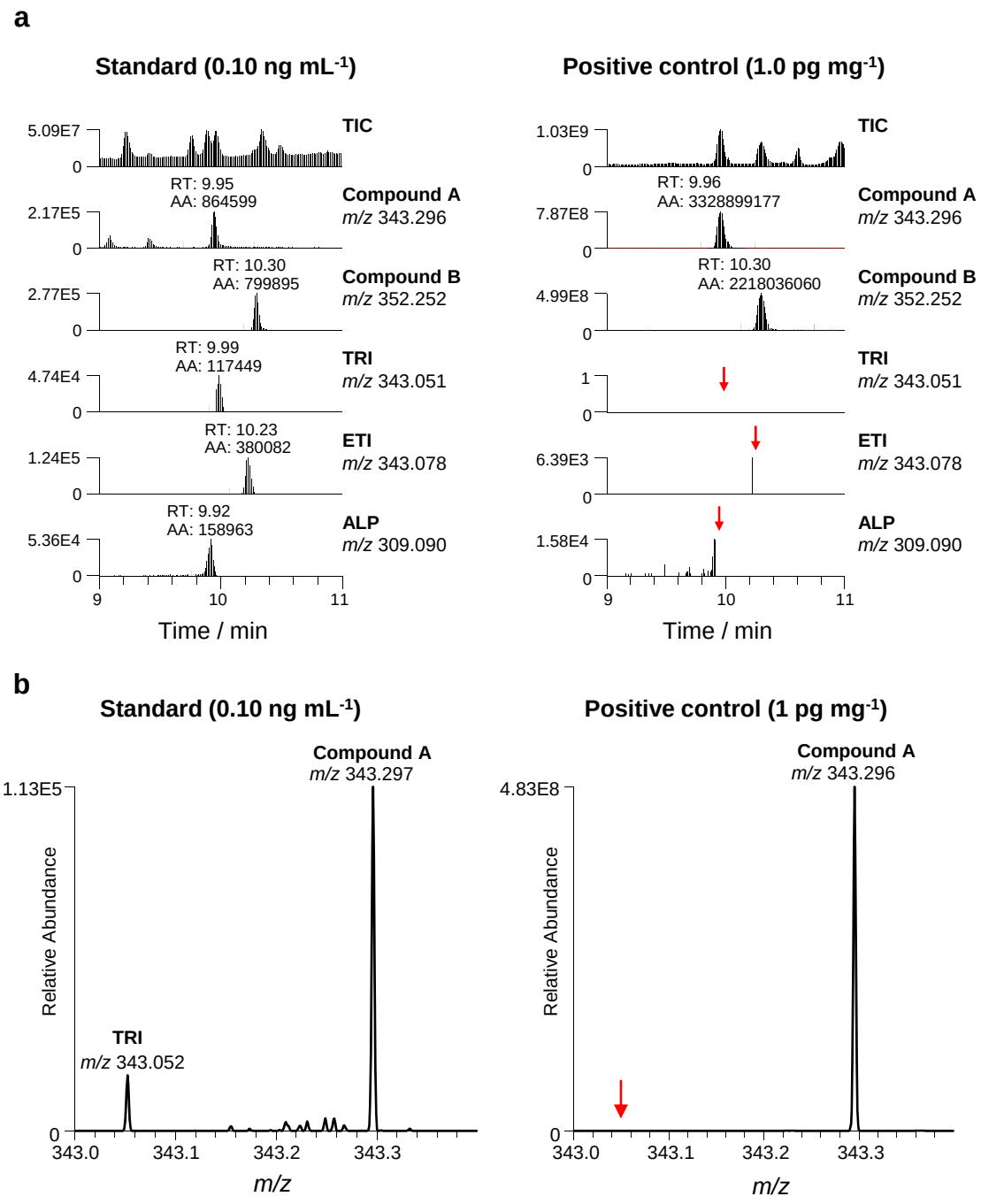

Fig. S1 Extracted ion chromatograms (a) and mass spectra (b) of the standard sample (0.10 ng mL^{-1}) and spiked sample (1.0 pg mg^{-1}).
Losses of small peaks of the analytes because of the limitations of the intra-scan dynamic range are indicated by arrows. The following conditions differed from the final protocol: mobile phase, 10 mol L^{-1} ammonium formate (A, pH 3.5)–acetonitrile (B) (0.3 mL/min); and gradient program, 0–2 min 10 % B, 2–8 min 10–90 % B, 8–15 min 90 % B, 15–20 min 10 % B.