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Corrigendum

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Corrigendum to "HighResNPS.com: An Online Crowd-Sourced HR-MS Database for Suspect and Non-targeted Screening of New Psychoactive Substances"

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In the Paper: "HighResNPS.com: An Online Crowd-Sourced HR-MS Database for Suspect and Non-targeted Screening of New Psychoactive Substances", the listed 'Acquisition control', 'Collision energies', and 'Scan range(s)' settings for the Agilent MassHunter screening in table II are incorrect. The correct acquisition control is: "DIA (AllIonsMS. Full-scan at four successive collision energies acquired over the 12 min chromatographic run. Scan rate at 5 spectra/sec, 0.8sec cycle time)", Collision energies: "0V, 10V, 20V, and 40V", and Scan range(s): "40-1,050".

The corrected Table II is reproduced here.

The authors regret the errors.

Table II. Experimental setups used in the participating laboratories for the HighResNPS data analysis

	Thermo Fisher TraceFinder	Waters UNIFI	Bruker Data analysis	Agilent MassHunter
LC system	Dionex Ultimate 3000 HPLC system (Thermo)	Acquity UPLC I-Class (Waters)	Acquity I-Class UPLC system (Waters)	1290 Infinity II LC system (Agilent)
LC column	Acquity UPLC 1.8 µm HSS C_{18} (150 mm x 2.1 mm) (Waters)	Acquity UPLC 1.8 µm HSS C_{18} (150 mm x 2.1 mm) (Waters)	Acquity UPLC 1.7 µm BEH C_{18}, (100 mm x 2.1 mm) (Waters)	Acquity 1.7 µm BEH C_{18} (50 × 3.0 mm) (Waters)
LC gradient	Linear gradient of 5-95 % B within 12.5 min. Mobile phase A: 2 mM ammonium formate buffer with 0.1 % formic acid (v/v). mobile phase B: 0.1 % formic acid in methanol (v/v)	Linear gradient of 13-50 % B from 0.5 to 10 min, then 50-95 % B from 10 to 10.75 min. Mobile phase A: 5 mM aqueous ammonium formate buffer (pH 3), mobile phase B: 0.1 % formic acid in acetonitrile (v/v)	Linear gradient of 0-20% B from 0 to 4 min, then 20-80% B to 8 min, constant 80% B to 8.5 min, 80-100% B to 9 min, constant 100%B to 10 min, and reequilibration at 0% B to 13.5 min. Mobile phase A: 0.1% aqueous formic acid, mobile phase B: acetonitrile	Linear gradient of 10-50 from 0.5-8 min, then 50-5% B from 8-10 min, constant for 0.1 min (with concurrent increase in flow rate to 400 µL/min), 0% B over 0.1 min and maintained for 1.8 min. Mobile phase A: 0.1% aqueous formic acid, mobile phase B: acetonitrile
Injection volume	1 µL	3 µL	10 µL	0.3 µL
Flow rate	200 µL/min	400 µL/min	600 µL/min	350 – 400 µL/min
Mass spectrometer type	Qq-Orbitrap	QqTOF	QqTOF	QqTOF
Trade name	Q-Exactive (Thermo)	Xevo G2-S QTof (Waters)	maXis Impact QTOF (Bruker)	6545 QTOF (Agilent)
Acquisition control	DDA (full-scan followed by MS/MS scan of top-5 signals with a dynamic exlusion of 5 s. Isolation width: 1 *m/z*)	DIA (MS scan at low and high collision energy; intensity threshold of 200 and 20 counts; deconvolution based on chromatographic coelution)	DIA (MS scan at low and high collision energy)	DIA (AllIonsMS. Full-scan at four successive collision energies acquired over the 12 min chromatographic run. Scan rate at 5 spectra/sec, 0.8sec cycle time)
Collision energy	NCE: 30 eV	LE: 4 eV HE: ramp from 10 to 40 eV	MS: 4 eV bbCID: 25 eV	0V, 10V, 20V, and 40V
Scan range(s)	MS 130-600, MS/MS dynamic first mass	50-950	50-1,000	40-1,050
Data analysis software	TraceFinder Forensic 4.1	UNIFI 1.8.2	Target Analysis (1.3) and Data Analysis (4.1)	MassHunter Quantitative Analysis (B.09) and MassHunter PCDL version B07

bbCID: broad-band collision induced dissociation, DDA: data-dependent acquisition, DIA: data-independent acquisition, HE: high energy, LC: liquid chromatography, LE: low energy, MS: mass spectrometry, MS/MS: tandem mass spectrometry, NCE: normalized collision energy