- Supporting Information -

The relevant role of ion mobility separation in LC-HRMS based screening strategies for contaminants of emerging concern in the aquatic environment

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Instrumentation

A Waters Acquity I-Class UPLC system (Waters, Milford, MA, USA) connected to a VION IMS-QTOF mass spectrometer, using electrospray ionisation (ESI) interface operating in both positive and negative ionisation mode was used for the analysis of samples. Chromatographic separation was performed using a CORTECS® C18 2.1 x 100 mm, 2.7 µm fused core column (Waters) at a flow rate of 300 µL min^{-1}. Gradient elution was performed using H_2O (A) and MeOH (B) as mobile phases, both with 0.01% formic acid. The initial percentage of B was 10%, which was immediately linearly increased to 90% over 14 min, followed by a 2 min isocratic period, and then returned to initial conditions (at 16.1 min) with a 2 min equilibration of the column. The total run time was 18 min. The injection volume ranged from 1 to 5 µL.

A capillary voltage of 0.8 kV for positive and 2.5 kV for negative ionization mode and a cone voltage of 40 V were used. The desolvation temperature was set to 550 °C, and the source temperature to 120 °C. Nitrogen was used as the drying gas and nebulizing gas. The cone gas flow was 250 L h^{-1} and desolvation gas flow of 1000 L h^{-1}. The column temperature was set to 40 °C and the sample temperature to 10 °C. MS data were acquired using the VION in HDMSe mode, over the range *m/z* 50-1000, with N_2 as the drift gas, an IMS wave velocity of 250 m s^{-1} and wave height ramp of 20-50 V. Leucine enkephalin (*m/z* 556.27658 and *m/z* 554.26202) was used for mass correction in positive and negative ionization modes, respectively. Two independent scans with different collision energies were acquired during the run: a collision energy of 6 eV for low energy (LE) and a ramp of 28-56 eV for high energy (HE). A scan time of 0.3 s was set in both LE and HE functions. Nitrogen (≥ 99.999%) was used as collision-induced dissociation (CID) gas. All data were examined using an in-house built accurate mass screening workflow within the UNIFI platform (version 1.9.4) from Waters Corporation.

Table S1. List of compounds spiked in water samples for the assessment of true/false identifications. Empirical CCS values for $[M+H]^+$ were obtained from standards and predicted CCS values were calculated using the predictive model developed by Bijlsma et al. Deviation was calculated between the empirical and the predicted CCS values.

Item Name	CCS Empirical (Å²)	CCS Predicted (Å²)	CCS dev (%)
2-hydroxy-terbuthylazine	153.11	148.80	-2.8%
4-Hydroxy omeprazole sulfide	174.93	170.97	-2.3%
Acetamiprid	152.21	144.71	-4.9%
Alprazolam	171.94	167.00	-2.9%
Atorvastatin	233.34	234.02	0.3%
Atrazine	149.26	144.41	-3.2%
Azithromycin	268.72	296.38	10.3%
Carbamazepine	149.11	150.89	1.2%
Carbaryl (Na adduct)	147.98	141.02	-4.7%
Chlorpyrifos (ethyl)	163.12	159.94	-1.9%
Ciprofloxacin (protomer I)	175.38	177.02	0.9%
Ciprofloxacin (protomer II)	188.89	177.02	-6.3%
Clarithromycin	271.25	273.66	0.9%
Clindamycin	202.49	201.92	-0.3%
Clothianidin	151.65	143.88	-5.1%
Deethylatrazine	139.64	134.07	-4.0%
Deethylterbumeton	146.07	143.32	-1.9%
Deisopropylatrazine	132.85	129.94	-2.2%
Desethyl terbuthylazine	144.71	138.21	-4.5%
Diclofenac	156.92	156.97	0.0%
Diuron	148.38	141.54	-4.6%
Enalapril	187.96	198.71	5.7%
Flumequine	150.58	153.44	1.9%
Furaltadone	173.06	173.84	0.4%
Gabapentin	139.70	134.98	-3.4%
Imazalil	166.56	166.24	-0.2%
Imidacloprid	153.91	150.24	-2.4%
Iopromide	223.51	210.15	-6.0%
Irbesartan	202.81	208.29	2.7%
Lincomycin	201.18	199.22	-1.0%
Linuron	151.01	145.45	-3.7%
Lorazepam	166.11	162.29	-2.3%
Losartan	200.49	201.85	0.7%
Metalaxyl	160.08	168.71	5.4%
Methiocarb sulfoxide	156.88	150.93	-3.8%
Metolachlor	159.39	166.56	4.5%

Item Name	CCS Empirical (Å^2)	CCS Predicted (Å^2)	CCS dev (%)
Metoprolol	172.54	170.78	-1.0%
Metronidazole	131.04	132.08	0.8%
Norfloxacin (protomer I)	171.88	174.12	1.3%
Norfloxacin (protomer II)	187.60	174.12	-7.2%
Pantoprazole	184.38	182.27	-1.1%
Paracetamol	130.56	128.67	-1.4%
Phenazone	135.59	138.04	1.8%
Primidone	147.25	146.56	-0.5%
Propamocarb	144.69	144.22	-0.3%
Pyridaphenthion	175.12	172.99	-1.2%
Roxithromycin	282.33	294.59	4.3%
Salbutamol	159.93	159.33	-0.4%
Simazine	143.00	139.26	-2.6%
Sulfadiazine	151.96	150.04	-1.3%
Sulfamethoxazole	152.61	150.42	-1.4%
Tebuconazole	166.80	173.06	3.8%
Terbumeton	156.21	155.14	-0.7%
Terbuthylazine	153.99	149.53	-2.9%
Terbutryn	160.48	156.97	-2.2%
Thiabendazole	137.44	133.11	-3.1%
Thiacloprid	156.97	146.74	-6.5%
Thiamethoxam	158.16	154.08	-2.6%
Tramadol	161.30	166.12	3.0%
Trimethoprim	172.89	170.14	-1.6%
Venlafaxine	171.86	171.31	-0.3%

Bijlsma, L., Bade, R., Celma, A., Mullin, L., Cleland, G., Stead, S., Hernandez, F., Sancho, J.V., 2017. Prediction of Collision Cross-Section Values for Small Molecules: Application to Pesticide Residue Analysis. Anal. Chem. 89, 6583–6589. https://doi.org/10.1021/acs.analchem.7b00741