Characterization and Separation of Platinum-Based Antineoplastic Drugs by Zwitterionic Hydrophilic Interaction Liquid Chromatography (HILIC)–Tandem Mass Spectrometry, and Its Application in Surface Wipe Sampling

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Table S1. Models coefficients computed and validation studied on six independent replicates of experiments in the point with coded coordinates (1, 1, 0.7, 0.6) corresponding to the experimental conditions selected for the analyses, i.e., mobile phase containing ACN 90% (v/v), ammonium formate 20 mM, pH 6.4, and column temperature set at 30 °C.

Rt	mean response	acn	fa	ph	t	acn*fa	acn*ph	acn*t	fa*ph	fa*t	ph*t	Predicted mean ± CI(95%)	Experimental mean ± CI(95%)	Conclusion
Cis	1.08	**0.15***	0.02	**0.09***	0.01	0.06	−0.03	0.00	−0.05	−0.04	**0.11***	1.34 ± 0.09	1.22 ± 0.02	Valid
Car	2.81	**0.97****	0.13	**0.62***	−0.25	0.36	−0.01	−0.13	−0.19	−0.3	**0.49**·	4.4 ± 0.5	4.2 ± 0.3	Valid
Oxa	1.42	**0.35****	0.04	**0.2***	−0.08	0.11	−0.02	−0.02	−0.08	−0.08	**0.19**·	2.0 ± 0.2	1.89 ± 0.09	Valid
W														
Cis	0.305	**−0.014****	0.000	0.002	**0.014***	0.002	−0.002	**−0.015****	−0.001	−0.001	0.002	0.292 ± 0.003	0.299 ± 0.002	Valid

LEGEND: column titles with lowercase letters refer to the factors considered in their coded values; acn, acetonitrile; fa, ammonium formate; t, column temperature; ph, pH. Rt, retention time models coefficients; W, model coefficient for peak width measured at half height of the peak. Cis, Cis-Pt; Car, Carbo-Pt; Oxa, Oxali-Pt.

Stars superscripts to the coefficient values refer to the statistical significance of the coefficient as tested by the Student t-test against the null hypothesis of having a coefficient value of 0. The coding for the p-values used is * significant at the 95% level of probability (0.01< p-value < 0.05), ** significant at the 99% level of probability (0.001< p-value < 0.01); *** significant at the 99.9% level of probability or more (p-value < 0.001)

Volume ratio calculation

$$V_W = (t_{R(ACN)} - t_{R(Phase)}) \times F$$
$$\beta = \frac{V_W}{V_{Phase}} = \frac{V_{ACN}}{V_{Phase}} - 1$$

Table S2. Shows the observed values from which was calculated the column volume ratio in the chromatography operating conditions.

$t_{R(Phase)}$ = 0.5085 min	V_{Phase} = 0.3051 mL
$t_{R(ACN)}$ = 0.5422 min	V_{ACN} = 0.32532 mL
Flow (F) = 0.6 mL/min	V_W = 0.02022 mL
β = 0.066273353	

LEGEND: $t_{R(Phase)}$, toluene retention time eluted with the mobile phase ACN 90%, H_2O 10% 20mM ammonium formate; $t_{R(ACN)}$, toluene retention time eluted with the mobile phase ACN 100%.

Table S3. Linear regressions data, R^2, LOD, and LOQ of each analyte.

	Interday				
Compound	**Slope (PAR/ng/mL)**	**Intercept (PAR)**	**R^2**	**LOD (ng/mL)**	**LOQ (ng/mL)**

Oxaliplatin	0.0112	0.0051	0.9982	1.6	4.8
Cisplatin	0.0012	0.0553	0.9977	78.9	236.6
Carboplatin	0.0113	0.0056	0.9986	1.5	4.4
		Intraday			
Oxaliplatin	0.0112	−0.0065	0.9996	0.8	2.5
Cisplatin	0.0015	0.0457	0.9988	58.0	174.0
Carboplatin	0.0099	−0.0047	0.9995	0.9	2.6

Table S4. Data results for matrix effect (ME) and recovery (RE).

Compound	ME	RE
Oxaliplatin	81%	82%
Cisplatin	94%	74%
Carboplatin	88%	79%

Table S5. Data results of precision and accuracy for the three CQI levels.

	Interday					
	Low		**Medium**		**High**	
	Precision (RSD %)	Accuracy (ratio %)	Precision (RSD %)	Accuracy (ratio %)	Precision (RSD %)	Accuracy (ratio %)
Oxali-platin	9%	95%	7%	99%	7%	99%
Cisplatin	6%	91%	7%	101%	5%	102%
Car-boplatin	7%	94%	5%	100%	8%	99%
	Intraday					
Oxali-platin	9%	111%	7%	100%	3%	103%
Cisplatin	6%	92%	5%	106%	4%	102%
Car-boplatin	7%	111%	3%	102%	4%	104%

Table S6. A simple scheme of positive results due to PtADs contamination on Laminar Flow Hood (LFH) surfaces in pg/cm^2.

Sampling Surface	Cisplatin	Carboplatin	Oxaliplatin
Working surface above the grid	<LOQ	31 pg/cm^2	76 pg/cm^2
Working surface under the grid	<LOD	< LOD	20 pg/cm^2
Prepared therapies storing box	<LOD	43 pg/cm^2	12 pg/cm^2
LFH control panel	<LOD	17 pg/cm^2	< LOD