Article

Developing a Fast Ultra-High-Performance Liquid Chromatography–Tandem Mass Spectrometry Method for High-Throughput Surface Contamination Monitoring of 26 Antineoplastic Drugs

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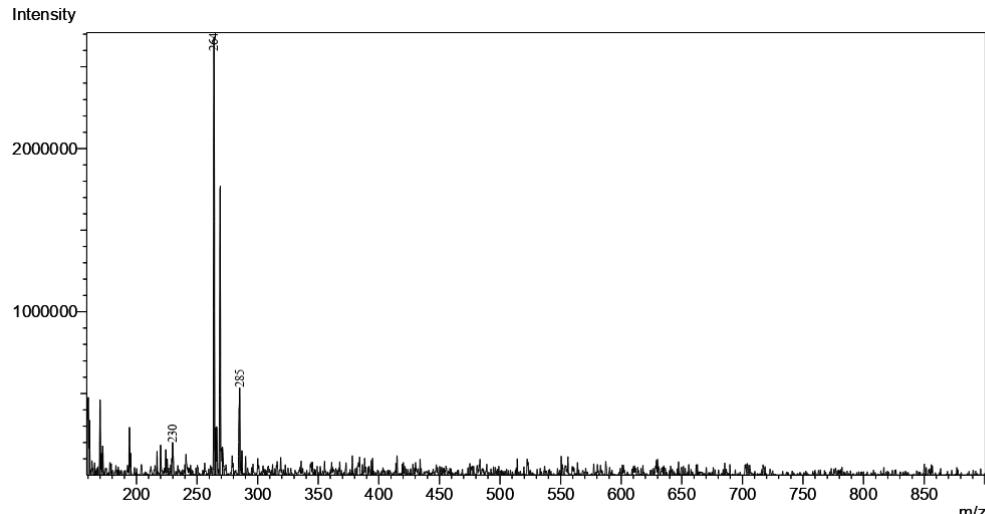
Figure S1. Busulfan mass spectrum obtained by scan mode.
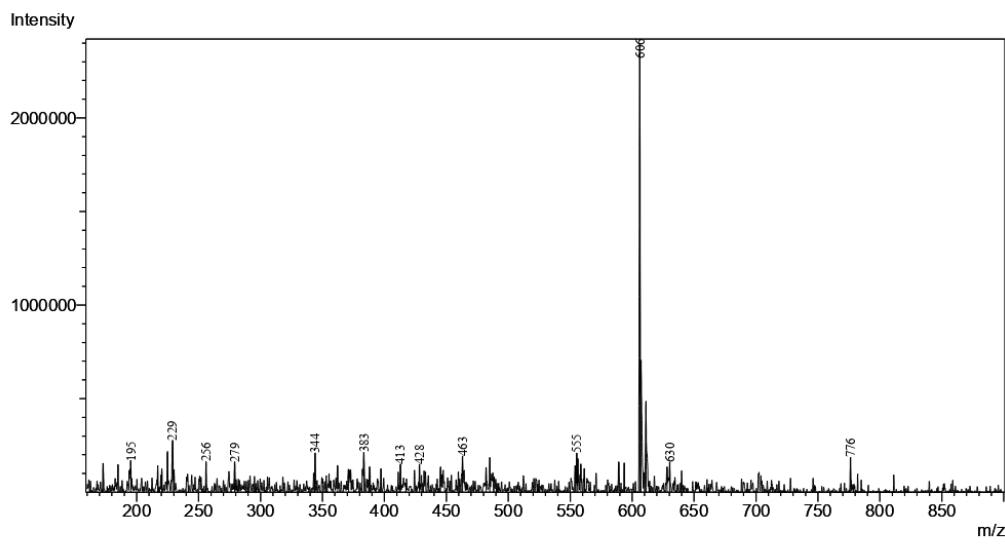
Figure S2. Etoposide mass spectrum obtained by scan mode.
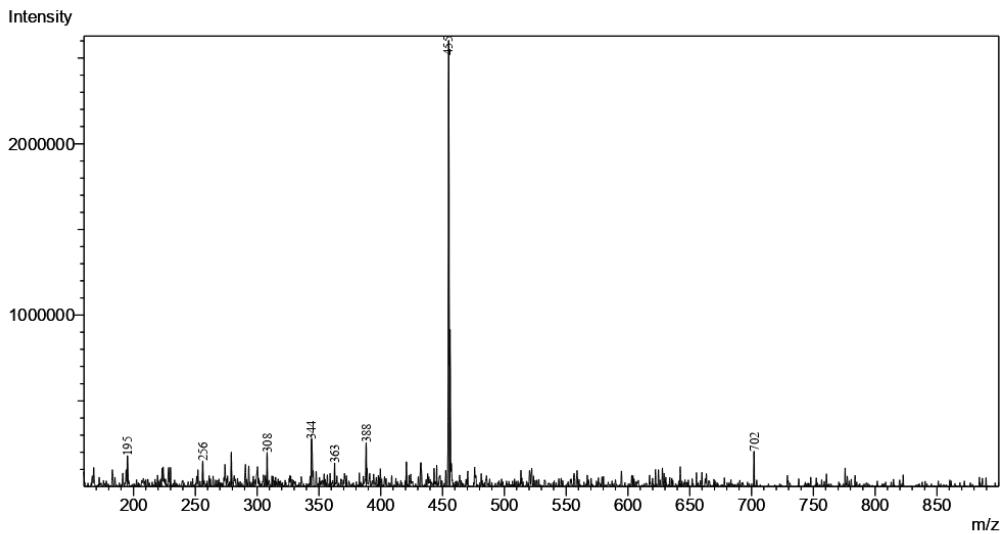
Figure S3. Methotrexate mass spectrum obtained by scan mode.
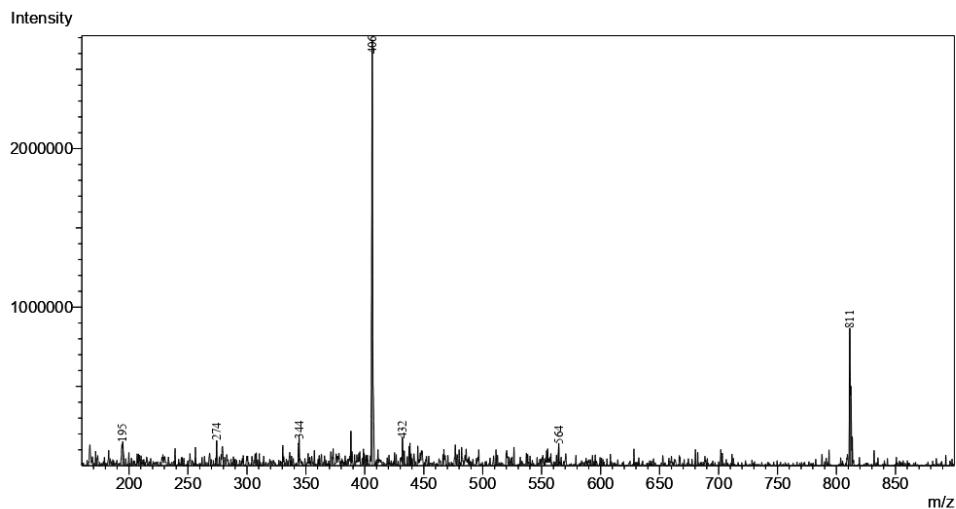
Figure S4. Vinblastine mass spectrum obtained by scan mode.
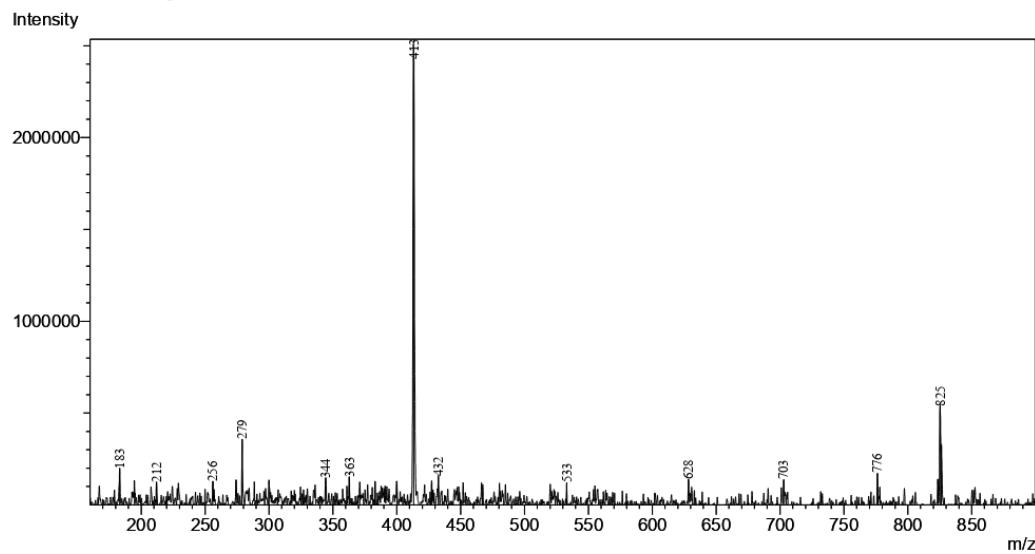
Figure S5. Vincristine mass spectrum obtained by scan mode.
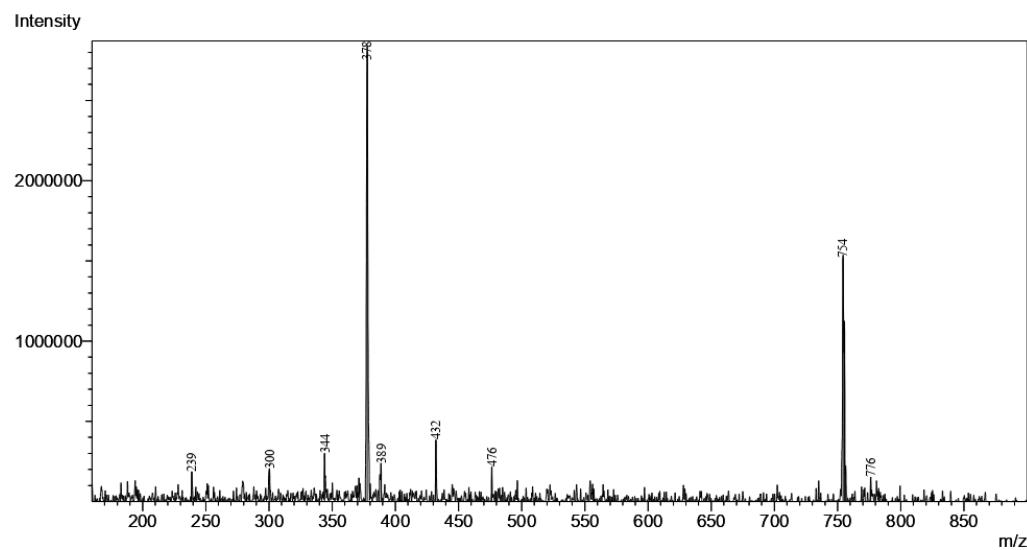
Figure S6. Vindesine mass spectrum obtained by scan mode.
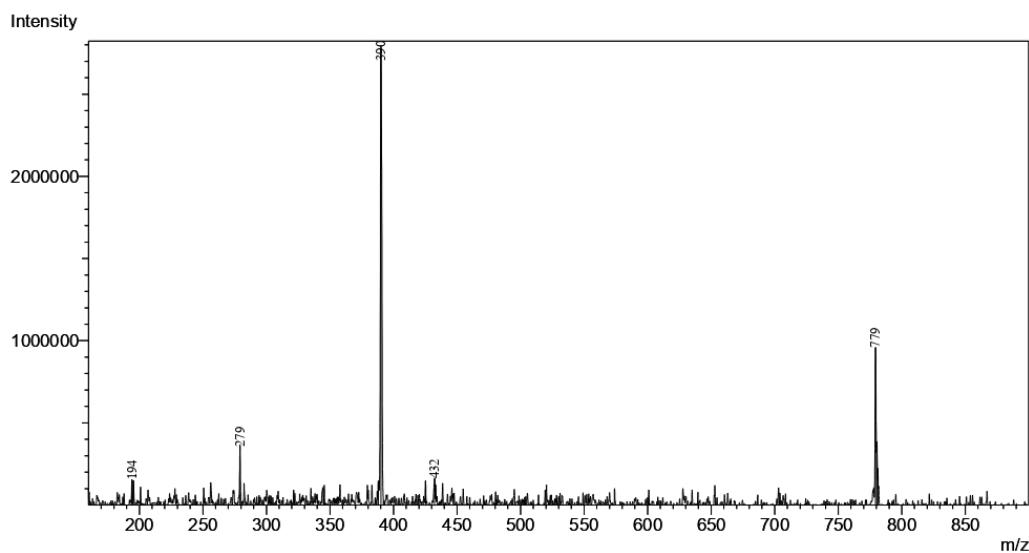
Figure S7. Vinorelbine mass spectrum obtained by scan mode.
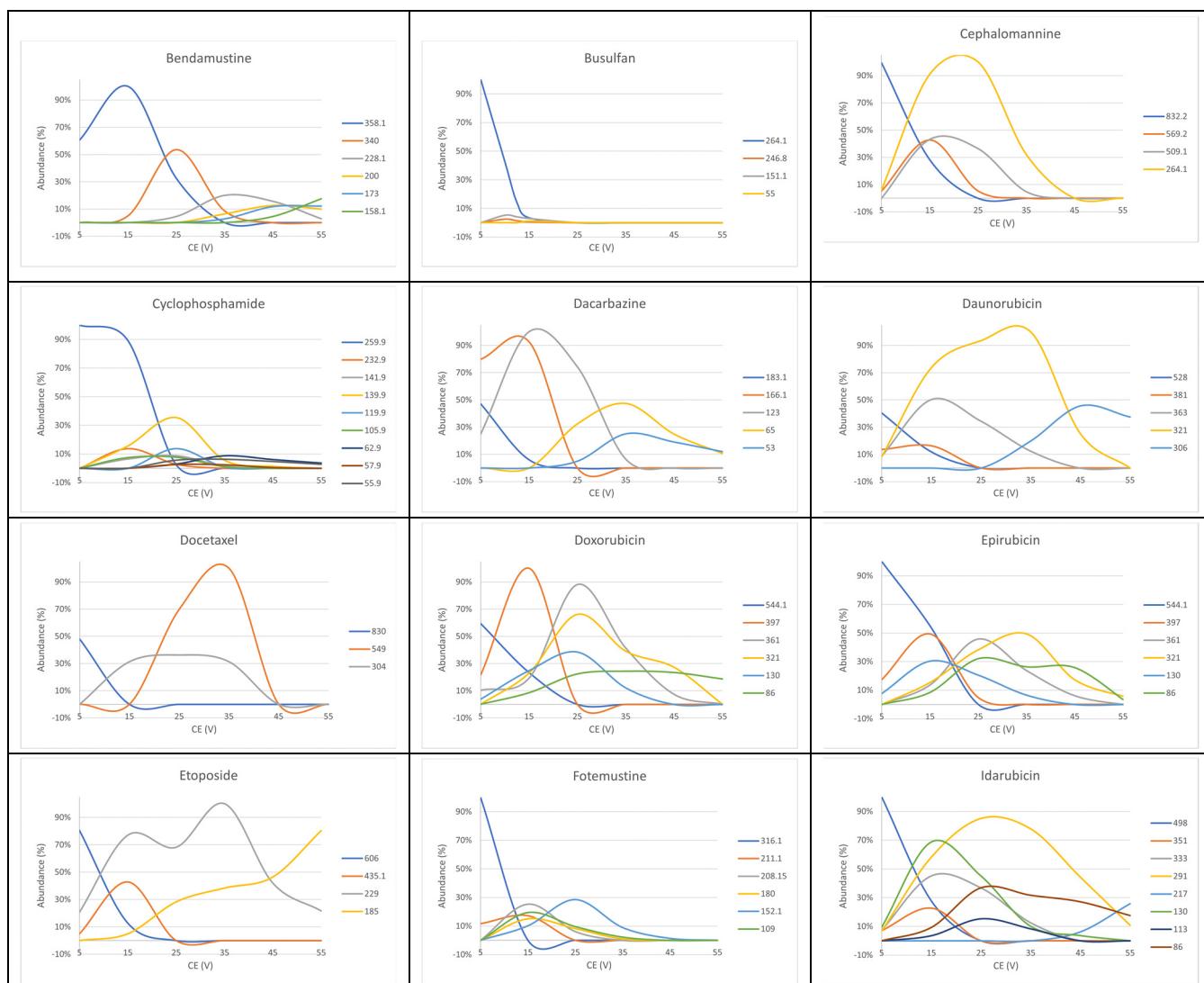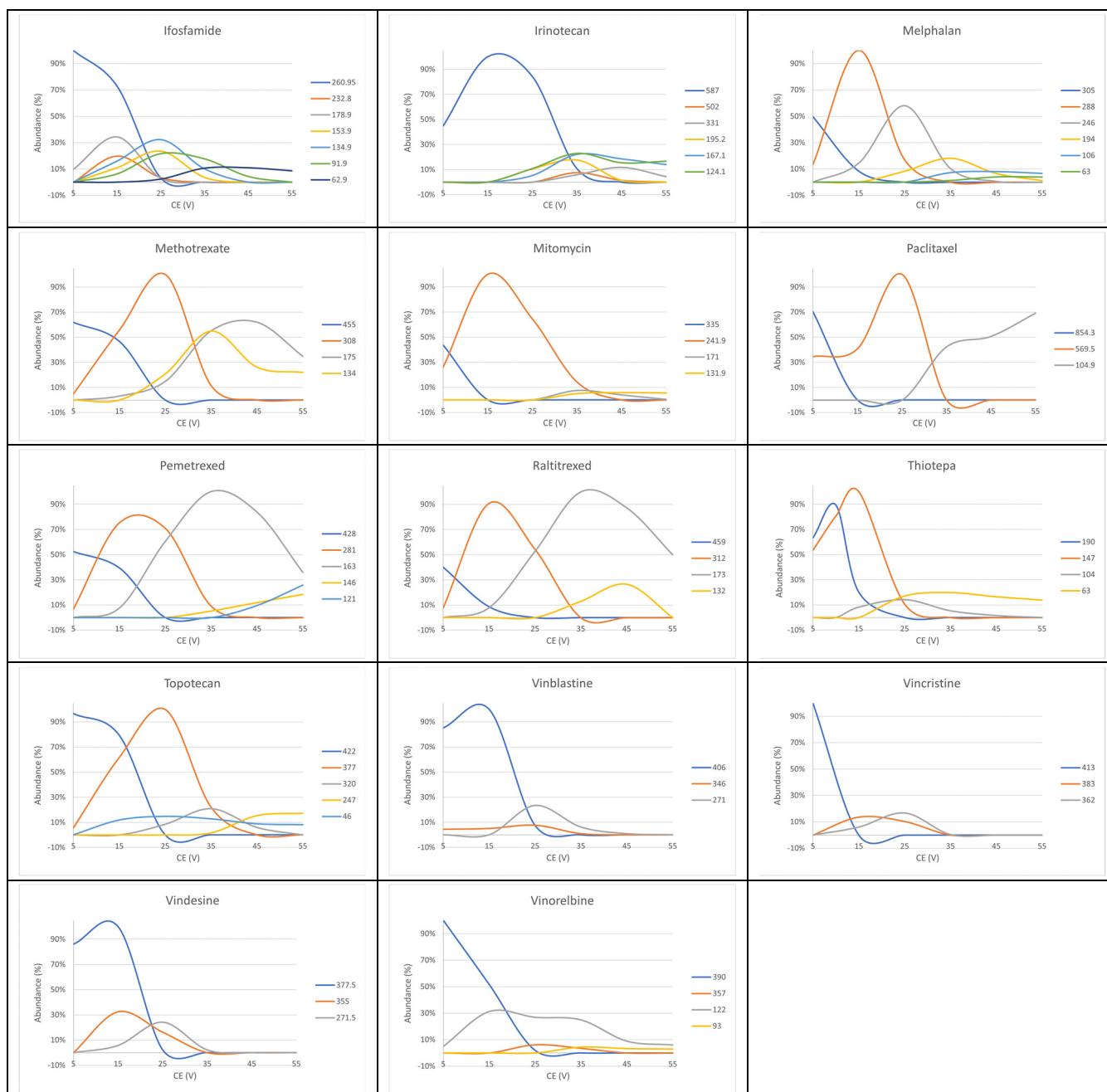
Figure S8. Collision breakdown curves obtained from PIS analysis reporting collision energy CE (V) versus percentage abundance. The listed values reported in each spectra legend are respectively precursor and product ions.

Table S1. Linear regression data, R^2, LOD, and LOQ of each analyte.

Compound	Slope (PAR/ng/mL)	Intercept (PAR)	R^2	LOD (ng/mL)	LOQ (ng/mL)
		Interday			
Fotemustine	2.066	-0.146	0.9981	0.010	0.036
Dacarbazine	3.793	-1.625	0.9972	0.014	0.044
Busulfan	0.325	0.581	0.9942	0.029	0.094
Methotrexate	11.539	1.669	0.9982	0.007	0.024
Mitomycin C	5.156	0.350	0.9977	0.005	0.017
Topotecan	4.790	-0.447	0.9978	0.010	0.034
Pemetrexed	0.404	0.093	0.9972	0.026	0.087
Vindesine	0.691	-1.480	0.9808	1.501	5.714
Raltitrexed	2.069	-2.013	0.9954	0.041	0.081
Ifosfamide	2.126	1.310	0.9975	0.011	0.035

Cyclophosphamide	3.127	1.885	0.9971	0.009	0.034
Irinotecan	1.053	-0.313	0.9968	0.016	0.055
Melphalan	0.105	0.006	0.9964	0.060	0.181
Vincristine	0.303	-0.132	0.9970	0.047	0.156
Vinblastine	0.063	-0.132	0.9914	0.136	0.440
Doxorubicin	0.159	0.004	0.9953	0.039	0.116
Etoposide	1.787	1.899	0.9967	0.067	0.213
Epirubicin	0.145	-0.022	0.9973	0.036	0.107
Vinorelbine	0.391	-0.210	0.9966	0.018	0.057
Daunorubicin	0.070	-0.044	0.9958	0.172	0.552
Idarubicin	0.039	-0.026	0.9953	0.206	0.618
Tamoxifen	0.296	-0.141	0.9981	0.028	0.075
Docetaxel	0.004	-0.003	0.9796	0.862	2.587
Paclitaxel	0.083	0.011	0.9963	0.062	0.185
Thiotepa	1.861	0.708	0.9976	0.014	0.046
Bendamustine	5.635	-2.576	0.9959	0.008	0.024
Intraday					
Fotemustine	1.980	-0.690	0.997	0.008	0.023
Dacarbazine	3.520	-2.155	0.996	0.007	0.022
Busulfan	0.291	0.488	0.997	0.069	0.206
Methotrexate	11.391	-0.271	0.997	0.005	0.014
Mitomycin C	4.755	-0.597	0.997	0.004	0.013
Topotecan	4.174	-0.760	0.997	0.007	0.021
Pemetrexed	0.353	0.242	0.998	0.044	0.133
Vindesine	0.643	-1.690	0.975	0.827	2.480
Raltitrexed	1.872	-1.298	0.992	0.070	0.210
Ifosfamide	1.877	0.989	0.996	0.004	0.011
Cyclophosphamide	2.809	1.472	0.995	0.007	0.021
Irinotecan	0.998	-0.452	0.993	0.020	0.060
Melphalan	0.090	0.010	0.994	0.064	0.193
Vincristine	0.282	-0.055	0.993	0.071	0.212
Vinblastine	0.057	-0.095	0.989	0.191	0.572
Doxorubicin	0.141	-0.018	0.995	0.066	0.197
Etoposide	1.581	1.850	0.998	0.087	0.262
Epirubicin	0.139	-0.063	0.993	0.144	0.431
Vinorelbine	0.363	-0.196	0.994	0.055	0.164
Daunorubicin	0.061	-0.037	0.995	0.325	0.974
Idarubicin	0.037	-0.030	0.994	0.070	0.209
Tamoxifen	0.352	-0.051	0.999	0.036	0.109
Docetaxel	0.004	0.001	0.992	0.746	2.239
Paclitaxel	0.071	0.005	0.993	0.066	0.198
Thiotepa	1.714	0.670	0.996	0.012	0.035
Bendamustine	5.498	-1.960	0.995	0.004	0.011

Table S2. Matrix effect values computed for each analyte.

CompoundTable Header	ME
Fotemustine	96%
Dacarbazine	95%
Busulfan	93%
Methotrexate	109%
Mitomycin C	92%
Topotecan	95%
Pemetrexed	96%
Vindesine	181%
Raltitrexed	102%
Ifosfamide	95%
Cyclophosphamide	95%
Irinotecan	95%
Melphalan	107%
Vincristine	89%

Compound	Value
Vinblastine	131%
Doxorubicin	96%
Etoposide	92%
Epirubicin	105%
Vinorelbine	94%
Daunorubicin	95%
Idarubicin	106%
Tamoxifen	86%
Docetaxel	342%
Paclitaxel	103%
Thiotepa	93%
Bendamustine	92%

Table S3. Precision and accuracy values computed for the three quality control levels.

	Interday					
	Low		**Medium**		**High**	
Compound	**Precision**	**Accuracy**	**Precision**	**Accuracy**	**Precision**	**Accuracy**
Fotemustine	5.8%	103.4%	5.6%	97.3%	5.8%	100.4%
Dacarbazine	5.2%	110.7%	4.0%	97.9%	5.7%	100.2%
Busulfan	5.5%	109.0%	5.8%	106.0%	6.2%	98.9%
Methotrexate	4.3%	110.1%	4.0%	104.1%	6.0%	102.6%
Mitomycin C	4.0%	109.7%	4.3%	104.3%	6.8%	101.1%
Topotecan	6.6%	109.0%	6.3%	100.3%	6.6%	100.4%
Pemetrexed	9.5%	109.1%	4.4%	105.6%	4.5%	102.4%
Vindesine	9.6%	113.9%	12.1%	83.1%	9.1%	88.2%
Raltitrexed	6.5%	106.3%	4.3%	101.8%	5.7%	105.4%
Ifosfamide	7.1%	109.0%	4.9%	101.7%	5.4%	101.2%
Cyclophosphamide	5.8%	106.2%	6.1%	101.8%	6.1%	102.9%
Irinotecan	5.6%	111.0%	5.6%	98.9%	4.9%	100.3%
Melphalan	8.6%	105.8%	6.6%	98.7%	6.2%	100.9%
Vincristine	7.3%	102.3%	6.5%	98.8%	7.5%	101.6%
Vinblastine	9.2%	102.3%	4.9%	96.0%	6.0%	100.1%
Doxorubicin	8.8%	106.4%	5.9%	98.0%	7.2%	96.6%
Etoposide	5.8%	110.4%	5.1%	105.4%	7.5%	104.0%
Epirubicin	5.9%	111.7%	5.6%	97.7%	7.0%	99.4%
Vinorelbine	7.2%	107.5%	4.7%	99.6%	5.2%	100.1%
Daunorubicin	6.0%	113.5%	5.3%	98.9%	6.8%	101.8%
Idarubicin	8.6%	106.1%	7.8%	94.4%	6.4%	101.3%
Tamoxifen	9.4%	97.8%	7.8%	101.9%	7.9%	98.2%
Docetaxel	21.7%	99.8%	14.0%	98.8%	13.2%	112.4%
Paclitaxel	10.5%	112.3%	4.2%	99.9%	6.7%	101.7%
Thiotepa	6.3%	107.2%	4.6%	100.2%	5.6%	99.2%
Bendamustine	10.2%	97.6%	7.5%	97.4%	8.5%	96.6%
	Intraday					
	Low		**Medium**		**High**	
Compound	**Precision**	**Accuracy**	**Precision**	**Accuracy**	**Precision**	**Accuracy**
Fotemustine	6.8%	101.9%	8.4%	95.6%	6.2%	100.2%
Dacarbazine	6.5%	108.0%	6.3%	96.4%	5.1%	96.8%
Busulfan	6.5%	109.0%	7.7%	99.9%	5.0%	97.4%
Methotrexate	5.6%	107.4%	5.7%	97.6%	3.0%	99.1%
Mitomycin C	7.5%	103.8%	3.2%	100.6%	3.5%	99.2%
Topotecan	10.9%	105.1%	6.4%	100.2%	6.4%	96.5%
Pemetrexed	8.3%	107.5%	5.2%	99.1%	3.4%	98.8%
Vindesine	7.3%	110%	19.1%	83%	11.0%	99%
Raltitrexed	9.1%	104.9%	4.7%	96.0%	2.8%	100.0%

Ifosfamide	9.4%	107.1%	6.9%	98.6%	4.7%	97.5%
Cyclophosphamide	8.1%	110.1%	7.6%	98.5%	3.6%	99.5%
Irinotecan	12.4%	109.6%	7.1%	97.1%	3.8%	97.9%
Melphalan	12.9%	104.9%	8.2%	100.9%	5.7%	96.0%
Vincristine	7.6%	107.8%	6.7%	96.2%	4.0%	95.5%
Vinblastine	6.8%	96.8%	6.1%	92.5%	4.5%	96.9%
Doxorubicin	9.2%	101.1%	6.6%	94.7%	3.6%	95.4%
Etoposide	8.0%	102.4%	5.4%	101.0%	4.4%	101.7%
Epirubicin	7.9%	103.6%	7.0%	93.3%	5.7%	97.4%
Vinorelbine	10.4%	105.7%	5.8%	95.1%	3.0%	97.9%
Daunorubicin	10.1%	110.8%	2.2%	91.1%	5.4%	97.1%
Idarubicin	6.9%	112.2%	14.5%	95.1%	5.1%	100.9%
Tamoxifen	11.3%	97.1%	7.1%	107.3%	8.5%	104.6%
Docetaxel	12.6%	103.3%	15.7%	93.9%	15.5%	101.3%
Paclitaxel	8.3%	105.0%	5.3%	96.3%	5.7%	99.0%
Thiotepa	11.1%	106.6%	7.6%	98.1%	5.9%	97.3%
Bendamustine	12.6%	104.2%	6.7%	105.0%	13.1%	95.5%