

Supporting Information

Quantitative analysis of multiple high-resolution mass spectrometry images using chemometric methods: Quantitation of chlordcone in mouse liver

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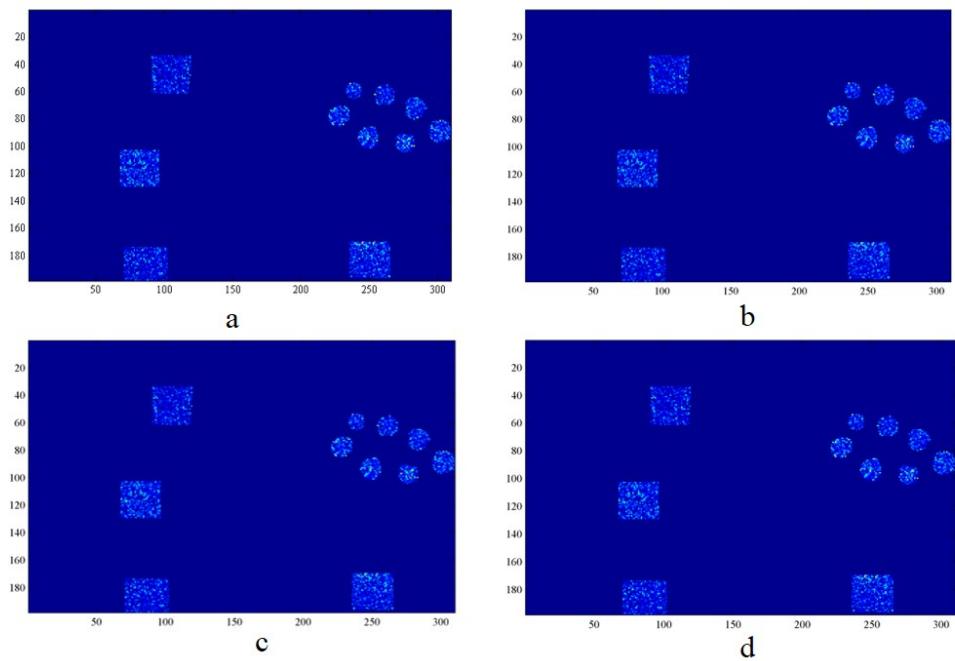


Figure S1. 2D image of (a) original data set II and binned data in (b) bin size 0.25 (c) bin size 0.5 (d) bin size 1

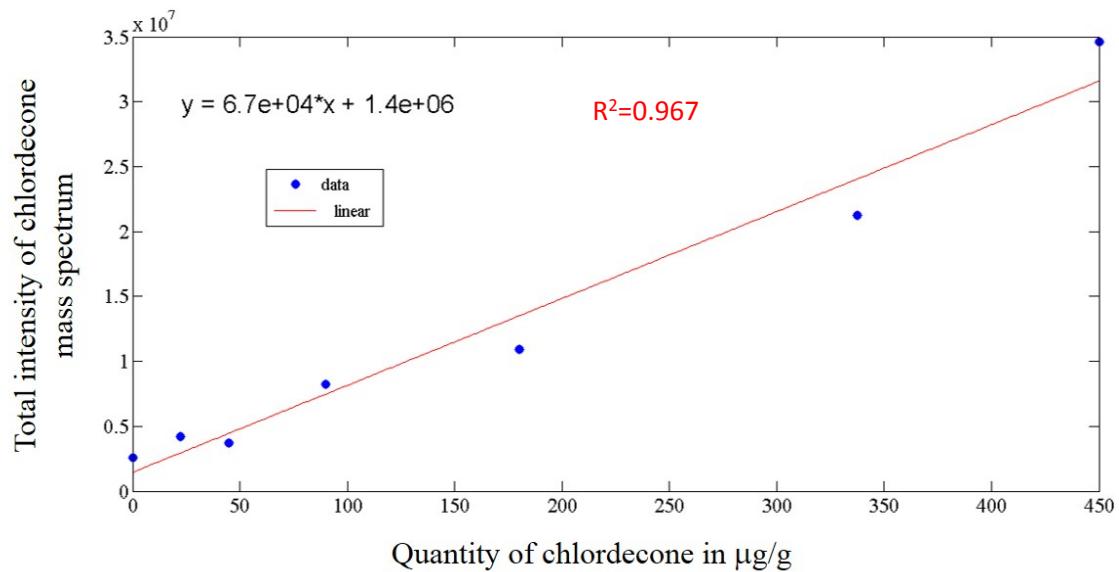


Figure S2. Calibration curve for data set II with bin size 0.25.

Table S1. Univariate analytical figures of merit for quantification of chlordecone using MALDI-MSI associated with MCR-ALS method.

	Slope			Intercept			LOF			RE (%) ^a		
Bin size Time (day)	0.25	0.5	1	0.25	0.5	1	0.25	0.5	1	0.25	0.5	1
1	2.6×10 ⁴	2.1×10 ⁴	1.6×10 ⁴	5.9×10 ⁶	1.2×10 ⁶	4.2×10 ⁵	4.1	5.3	10.7	10.3	11.2	8.37
5	6.7×10 ⁴	2.5×10 ⁴	4.2×10 ⁵	2.8×10 ⁵	4.7×10 ⁶	1.2×10 ⁶	7.0	7.5	11.7	6.5	8.2	11.2
10	7.0×10 ⁴	4.2×10 ⁴	3.0×10 ⁴	1.3×10 ⁶	2.8×10 ⁵	4.8×10 ⁶	7.0	8.3	8.4	3.8	6.5	6.99

$$^a \text{RE}(\%) = 100 \sqrt{\frac{\sum_i (ci - \hat{ci})^2}{\sum_i (ci)^2}}$$