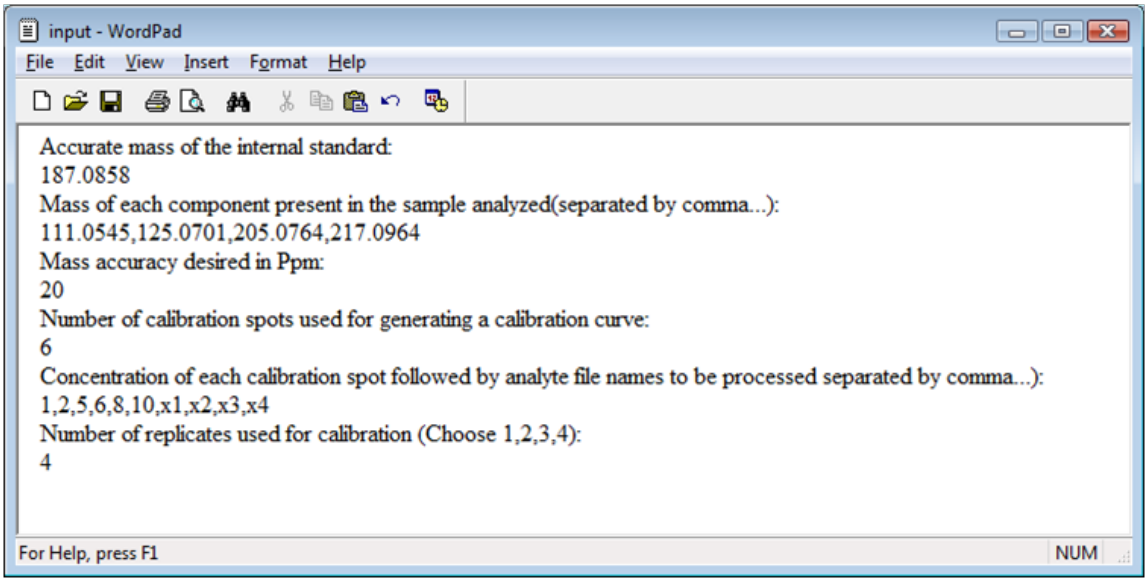
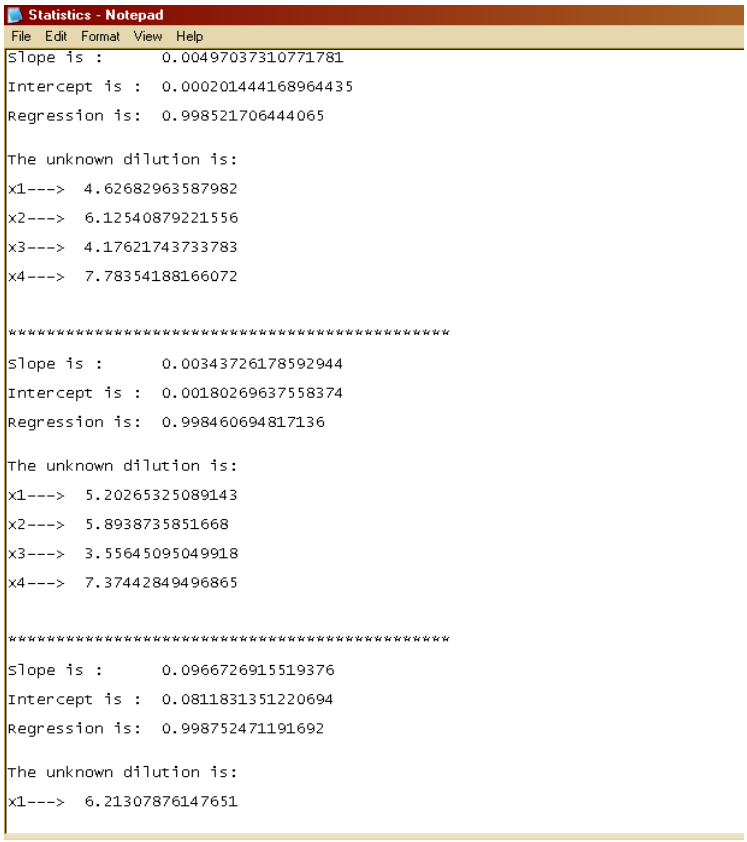
Electronic Supplementary Material (ESI) for Analytical Methods

Supporting information and figures

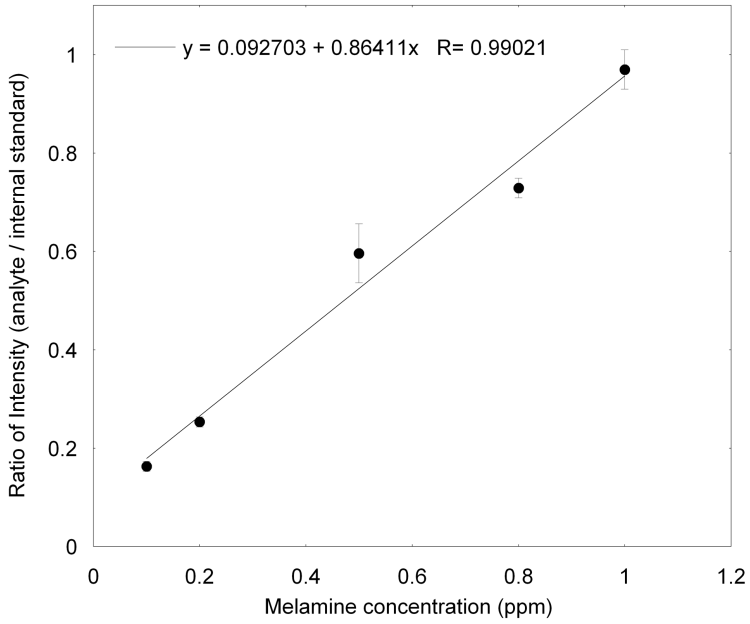
Algorithm for high throughput MALDI MS data processing and quantitation

For the mass spectral data analysis using 'MQ' software, all the spectra were converted into ASCII files containing *m/z* and absolute signal intensities using the manufacturer's software. An algorithm to process these files was coded in Perl script. Screen shots for the input files and the resulting output are shown in supplementary information (Supplementary figure 1). Typically, the input file specifies the number of calibration points, corresponding concentrations, replicates, number of components along with a choice of adducts and the desired level of mass accuracy. Peaks are subsequently picked from data files based on the highest intensities for each of the components within the mass accuracy in ppm specified by the user. Following the selection of the analyte(s) as well as the internal standard peaks, the calibration curves are generated (analyte: IS ratio Vs concentration) and the unknown concentration determined. A linear regression using least square fitting is then enforced to output the linearity performance as represented by the mean slope, intercept and R-squared values for each of the components. Quantitation obtained using the MQ algorithm was thoroughly verified using manual quantitation for both the s-triazine and melamine analysis before implementing it for the high throughput workflows.





Supplementary figure 1. Typical 'MQ' input file and output screenshots.



Supplementary figure 2. Concentration response curve for melamine standard showing linearity (R 0.99) in the range of 0.1 ppm to 1 ppm obtained using MALDI MS.

Concentration	Analyte 1	Analyte 2	Analyte 3	Analyte 4
5 ppm	20.36	-2.28	-0.84	-4.75
6 ppm	7.81	2.08	-12.82	-9.90
2 ppm	0.81	-22.53	-33.83	-28.78
8 ppm	-21.53	-59.19	1.46	-2.25

Supporting figure 3. Average percentage errors obtained in the high throughput analysis of triazine mixture components shown in figure 4. The error percentages were averaged for various spots at different locations on the MALDI target plate containing an identical concentration of the individual analytes 1 through 4.