

## Supporting Information

*J. Chem. Metrol.* 14:1 (2020) 63-68

### Determination of doxylamine from a tea sample: A claim of drug facilitated crime

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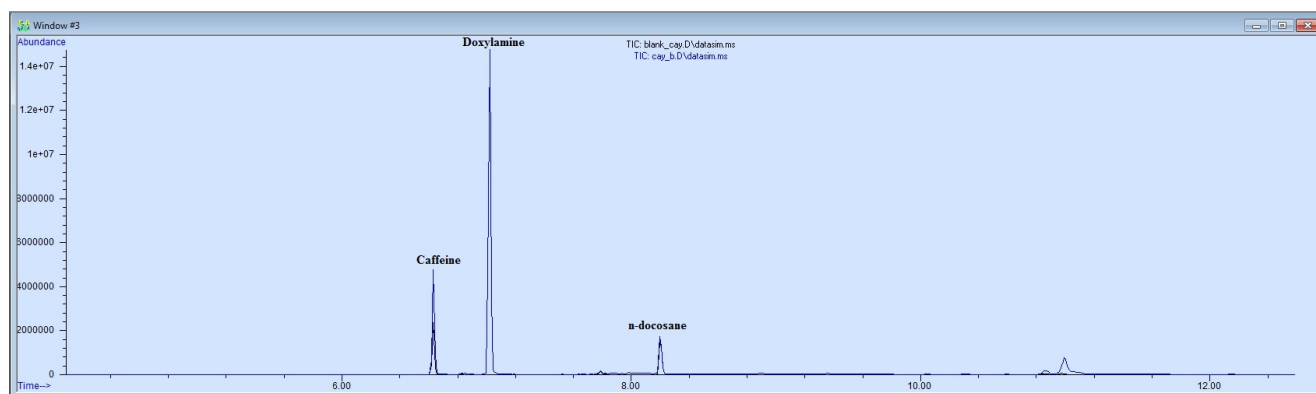
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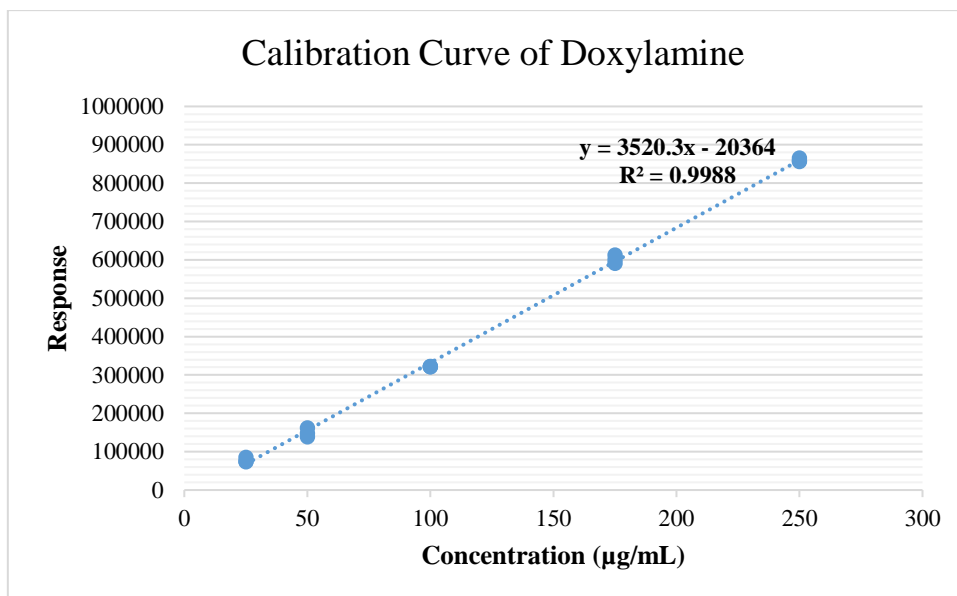
## S1. Validation Studies of Quantitative Method

A quantitative analysis method was developed to quantify the doxylamine level detected in the systematic toxicological screening result of the sample. For the quantitative analysis of doxylamine, several analytical performance parameters such as linearity, limit of detection (LOD), limit of quantitation (LOQ), recovery, precision and repeatability were investigated. Five-step calibration solutions were prepared with incremental concentrations of 25, 50, 100, 175, 250  $\mu\text{g/mL}$  and each calibration points were analyzed in triplicate. Calibration curve was generated by linear regression method as shown in Fig. S2. In the mass spectrum of the doxylamine substance, selected ions ( $m/z$  58, 71, 167, 180) were monitored.

To verify the developed method and mimic the case, commercially available tea bags were bought and validation studies were conducted by spiking into hot tea samples. Also, a blank tea sample, only spiked with IS, was extracted and analyzed to check out the matrix effect. Recovery studies were conducted with two different concentrations of doxylamine (50 and 175  $\mu\text{g/mL}$ ). Studies were repeated three times for each recovery point and samples were extracted as mentioned in sample preparation section. Precision and repeatability of the method were evaluated considering the results by calculating standard deviation (SD) and relative standard deviation (RSD%) values. LOD level was assumed as three times the noise level ( $S/N:3$ ) while LOQ was ten times ( $S/N:10$ ). Mean, SD, RSD% and recovery values (%) of the findings were calculated in Windows-based Excel program.



**Figure S1:** Overlaid chromatograms of blank tea and questioned tea samples



**Figure S2:** Calibration curve of doxylamine.

**Table S1:** Analytical results of the validated GC-MS method

Linear regression equation	Linear range (µg/mL)	r <sup>2</sup>	Recovery %	LOD/LOQ (µg/mL)	RSD%
y = 3520.3x - 20364	25-250	0.999	97.5% at 50 µg/mL (n=3) 85.6% at 175 µg/mL (n=3)	1.35 / 4.46	≤6.29

r<sup>2</sup>: Correlation coefficient

**Ethical declaration:** Biological material was not used; personal data were not shared in this study. In addition, the complainant was informed about scientific publication and technical process, and signed the informed consent form. The editor of the journal has also been informed and a signed declaration of ethical status is provided to Publisher.