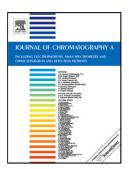
Accepted Manuscript

Title: Determination of nitroalkanes in mainstream cigarette smoke by heart-cutting multidimensional gas chromatography system coupled with mass spectrometry detection



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PII:	S0021-9673(15)01566-6
DOI:	http://dx.doi.org/doi:10.1016/j.chroma.2015.10.078
Reference:	CHROMA 356993
To appear in:	Journal of Chromatography A
Received date:	25-8-2015
Revised date:	26-10-2015
Accepted date:	26-10-2015

Please cite this article as: X. Wang, J. Guo, J. Shang, L. Ding, G. Zhao, F. Xie, Y. Jia, Y. Qin, Y. Yu, L. Chen, S. Zhang, Determination of nitroalkanes in mainstream cigarette smoke by heart-cutting multidimensional gas chromatography system coupled with mass spectrometry detection, *Journal of Chromatography A* (2015), http://dx.doi.org/10.1016/j.chroma.2015.10.078

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ACCEPTED MANUSCRIPT

- 1 Determination of nitroalkanes in mainstream cigarette smoke by heart-cutting multidimensional
- 2 gas chromatography system coupled with mass spectrometry detection
- 3 4
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- 12
- 13
- 14 Highlights
- 15 A GC-GC/MS method was developed and validated for the determination of 6 16 nitroalkanes in mainstream cigarette smoke.
- 17 The home-made double oven GC-GC/MS equipment used could realize 18 cryo-concentration at the inlet of the second column.
- 19 The GC-GC/MS method exhibited higher sensitivity and lower noise than GC/MS.
- 20 The method required only a simple vapor phase collection step before injection.
- The GC-GC/MS method avoided the false positive/negative results that appeared in GC/MS.
- 23

24 ABSTRACT

25 In this paper, heart-cutting two-dimensional GC/MS (GC-GC/MS) method in 26 combination with a simple sample collection procedure was developed for the determination of 6 nitroalkanes in mainstream cigarette smoke. The method could 27 28 remove large amounts of impurities on-line in the first polar column by heart-cuts and 29 separate from the left interferences in a second mid-polar column. And the target 30 compounds could be focused at the inlet of the second column by cryo-concentration. Compared to conventional GC/MS, GC-GC/MS achieved a lower noise level and 31 sensitivity at least an order of magnitude higher. Furthermore, the GC-GC/MS method 32 33 could avoid the false negative and false positive results that appeared in the compared 34 conventional GC/MS analysis. By trapping the vapor phase of 20 cigarettes smoke, 35 the LODs and LOQs of the nitroalkanes were 1.3 to 9.8 and 4.3 to 32.6 ng/cigarette, 36 respectively, and all linear correlation efficiencies were larger than 0.999. The 37 validation results also indicate that the method has high accuracy (spiked recoveries 38 between 84% and 102%) and good repeatability (RSD between 7.2% and 9.4%). The 39 developed method was applied to analyze 1 Kentucky reference cigarette (3R4F) and 40 10 Chinese commercial brands of cigarettes. The research results indicated that 41 nitromethane, nitroethane, 2-nitropropane and 1-nitro-n-pentane were detected in 42 mainstream cigarette smoke, but 1-nitro-n-butane and 2-nitropropane, which were 43 reported by one previous study, were not detected in all cigarette samples.

44 Keywords: Heart-cut; Two-dimensional GC; Cold trap; Mainstream smoke;

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