

1 **SUPPLEMENTARY MATERIAL**

2 **Quantification of Twenty-one Metabolites of Methylnaphthalenes and Polycyclic Aromatic**
3 **Hydrocarbons in Human Urine**

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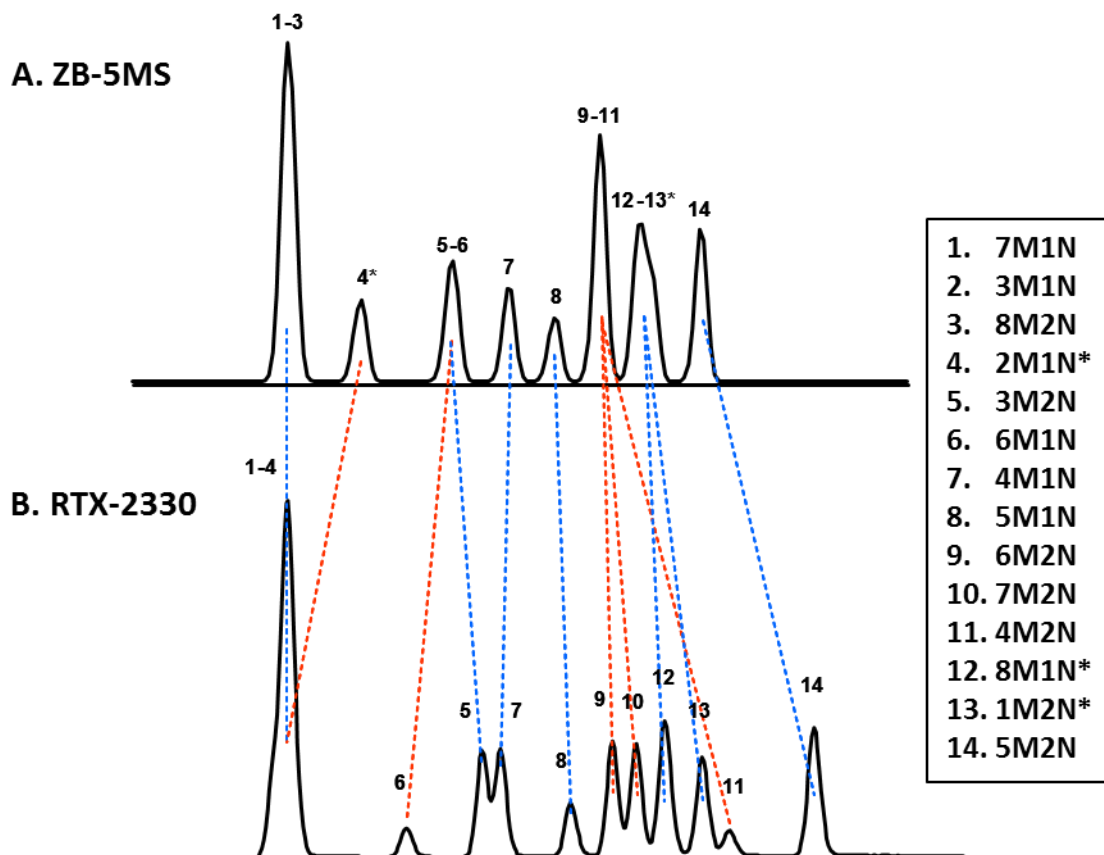
1 **Accurate mass peak profiling for peak confirmation**

2 Identity of the Me-OHN peaks in urine samples was confirmed by the use of mass peak profiling
3 (Grant et al., 1994) at mass resolution of 10,000 on a magnetic sector high-resolution mass
4 spectrometer (MAT95XL, Thermo Fisher Scientific Inc. Waltham, MA, USA). The calculated
5 exact mass for the molecular ion and 16 additional masses, 8 on each side of the exact mass at an
6 increment of 10 ppm, were monitored as the capillary GC peaks eluted. Mass profiles were
7 constructed by plotting ion abundance as a function of mass. The apex of the mass profiles in a
8 urine sample matched the exact mass and that from a standard, confirming the identity of the
9 Me-OHN peaks.

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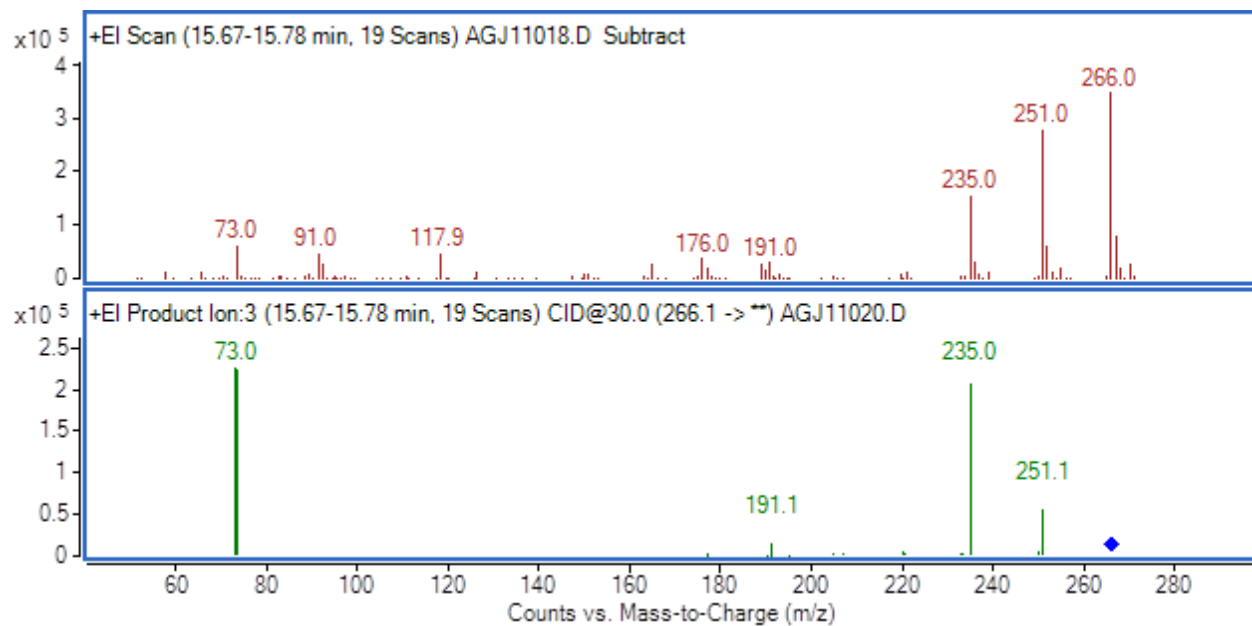
11 Reference:

12 Grange AH, Donnelly JR, Brumley WC, Billets S, Sovocool GW. (1994) Anal Chem. 66:4416-
13 4421

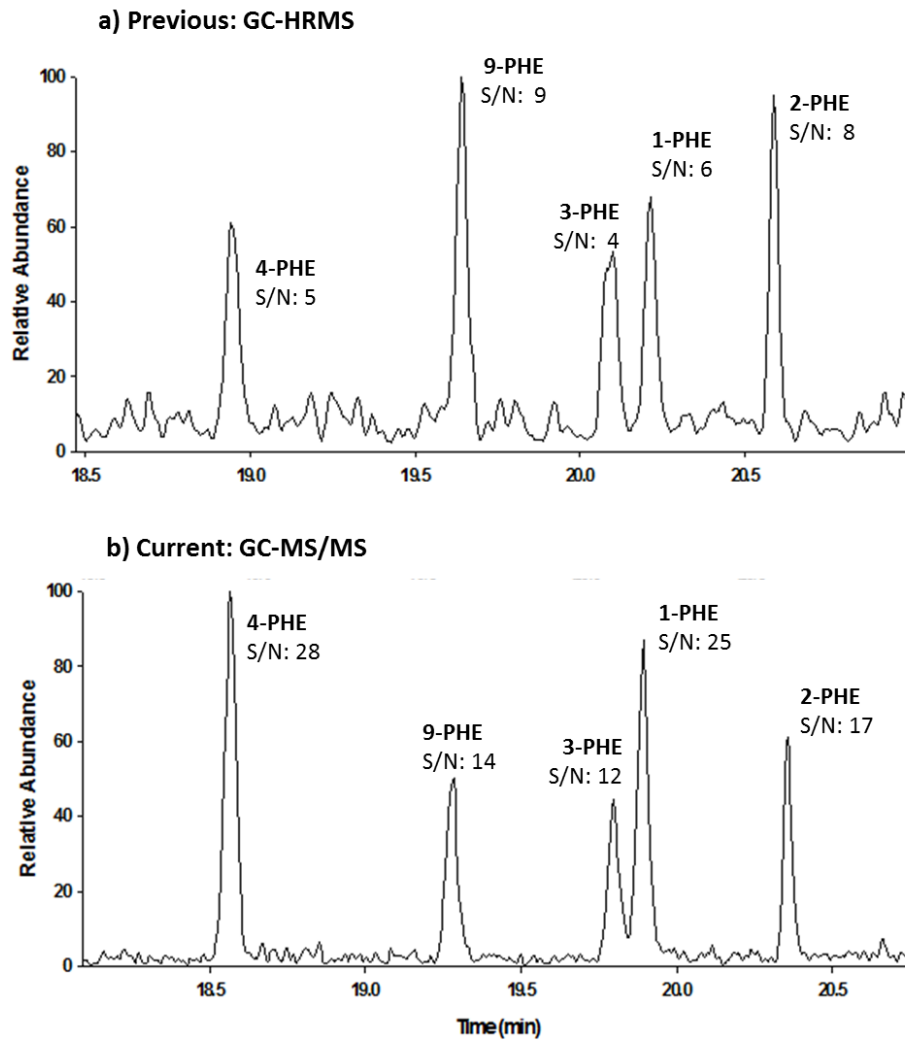


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 2 Figure S1. GC chromatograms of 14 methyl naphthols on (A) a non-polar ZB-5MS column and
 3 (B) a polar Rtx-2330 column. Peaks represent the trimethylsilyl ethers of OH-PAHs and Me-
 4 OHNs. Peaks marked with an asterisk are isomers that are not reported in this method.

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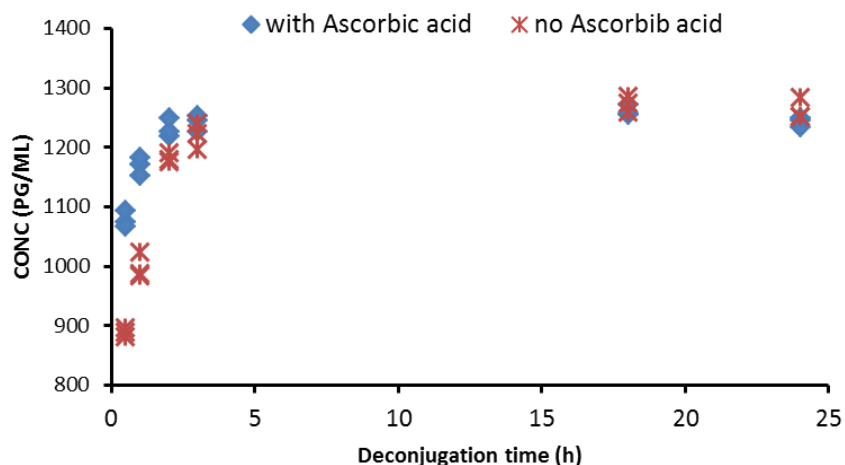


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2 Figure S2. A full scan spectrum of the trimethylsilyl ether of 1-hydroxyphenanthrene (top) and a
3 product ion scan of its molecular ion (bottom).

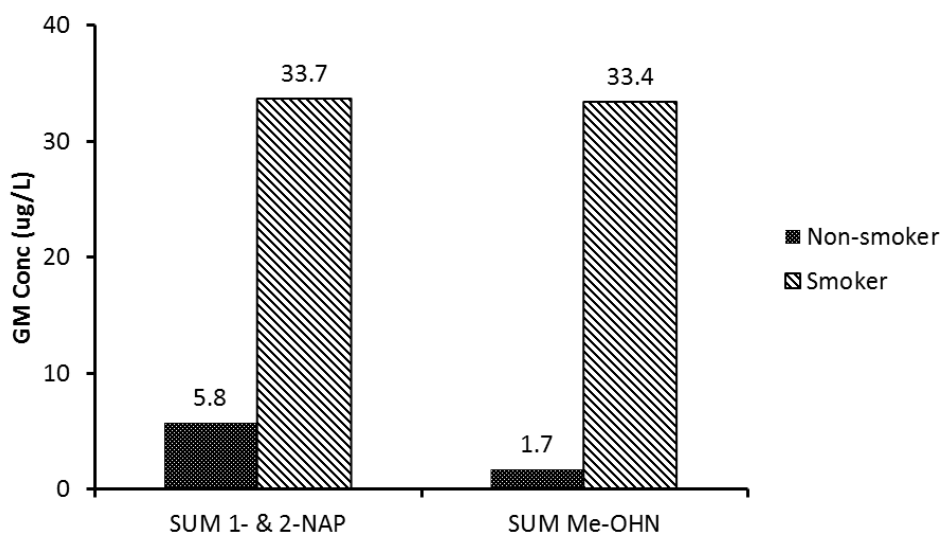


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 2 Figure S3. GC chromatograms of the lowest calibration standard (25 fg on column) from the
 3 previous method using GC high resolution mass spectrometry (GC-HRMS) (a) and the current
 4 method using GC-MS/MS (b). Peaks represent the trimethylsilyl ethers of OH-PAHs and Me-
 5 OHNs.

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 2 Figure S4. Calculated concentrations of 9-hydroxyfluorene in a smoker's urine sample as a
 3 function of deconjugation time (1, 2, 3, 18 and 24 h), with or without ascorbic acid (2.5 mg/mL
 4 urine) during hydrolysis.



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 7 Figure S5: Geometric mean concentrations of summed 1- and 2-naphthols (metabolites of
 8 naphthalene) and summed methyl naphthols (metabolites of 1- and 2-methylnaphthalene) in 30
 9 smokers and 30 non-smokers.