**Analytical and Bioanalytical Chemistry**

**Electronic Supplementary Material**

# Silicone wristbands compared with traditional polycyclic aromatic hydrocarbon exposure assessment methods

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## Chemical Information for Wristband Methodology

We purchased PAH standards from Sigma Aldrich (St. Louis, MO), Accustandard (New Haven, CT), and Chiron (Trondheim, Norway). All solvents were Optima-grade or equivalent (Fisher Scientific, Pittsburgh, PA). All of the glassware and tools used were baked for 12 hours at 450°C and/or solvent-rinsed before use. Eighteen MΩ*cm water used to clean silicone was filtered through a D7389 purifier (Barnstead International, Dubuque, IA).

## Additional CDC Quality Control Details

The CDC laboratory is certified by the Health Care Financing Administration to comply with the requirements set forth in the Clinical Laboratory Improvement Act of 1988 (CLIA '88) and is recertified every two years. At CDC, analytical measurements are conducted following strict quality control/quality assurance CLIA guidelines, and include participation in external quality assessment schemes to continuously demonstrate the accuracy and precision of CDC's analytical methods.

**Table S1** PAH surrogates and target compounds in wristband analysis method

| PAH | Molecular Weight ($g\ mol^{-1}$) | Target, Internal Standard (IS), or Surrogate | PAH | Molecular Weight ($g\ mol^{-1}$) | Target, Internal Standard (IS), or Surrogate |
|---|---|---|---|---|---|
| Perylene-d12 | 264.34 | IS | Benzo[a]fluorene | 216.23 | Target |
| Naphthalene-d8 | 136.22 | Surrogate | Benzo[b]fluorene | 216.23 | Target |
| Acenaphthylene-d8 | 160.25 | Surrogate | Benzo[c]fluorene | 216.23 | Target |
| Phenanthrene-d10 | 188.30 | Surrogate | 1-Methylpyrene | 216.28 | Target |
| Fluoranthene-d10 | 212.31 | Surrogate | Benz[a]anthracene | 228.29 | Target |
| Chrysene-d12 | 240.36 | Surrogate | Cyclopenta[c,d]pyrene | 229.27 | Target |
| Benzo[a]pyrene-d12 | 264.39 | Surrogate | Triphenylene | 228.29 | Target |
| Benzo[ghi]perylene-d12 | 288.41 | Surrogate | Chrysene | 228.28 | Target |
| Naphthalene | 128.17 | Target | 6-Methylchrysene | 242.31 | Target |
| 2-Methylnaphthalene | 142.20 | Target | 5-Methylchrysene | 242.31 | Target |
| 1-Methylnaphthalene | 142.20 | Target | Benzo[b]fluoranthene | 252.30 | Target |
| 2-Ethylnaphthalene | 156.09 | Target | 7,12-Dimethylbenz[a]anthracene | 256.34 | Target |
| 2,6-Dimethylnaphthalene | 156.22 | Target | Benzo[k]fluoranthene | 252.30 | Target |
| 1,6-Dimethylnaphthalene | 156.22 | Target | Benzo[j]fluoranthene | 252.30 | Target |
| 1,4-Dimethylnaphthalene | 156.22 | Target | Benz[j]&[e]aceanthrylene | 256.31 | Target |
| 1,5-Dimethylnaphthalene | 156.22 | Target | Benzo[e]pyrene | 252.30 | Target |
| 1,2-Dimethylnaphthalene | 156.22 | Target | Benzo[a]pyrene | 252.30 | Target |
| 1,8-Dimethylnaphthalene | 156.22 | Target | Indeno[1,2,3-c,d]pyrene | 276.33 | Target |
| 2,6-Diethylnaphthalene | 184.27 | Target | Dibenzo[a,h]pyrene | 278.35 | Target |
| Acenaphthylene | 152.19 | Target | Picene | 278.35 | Target |
| Acenaphthene | 154.20 | Target | Benzo[ghi]perylene | 276.33 | Target |
| Fluorene | 166.22 | Target | Anthanthrene | 276.33 | Target |
| Dibenzothiophene | 184.26 | Target | Naphtho[1,2-b]fluoranthene | 302.36 | Target |
| Phenanthrene | 178.23 | Target | Naphtho[2,3-j]fluoranthene | 302.36 | Target |
| Anthracene | 178.23 | Target | Dibenzo[a,e]fluoranthene | 302.37 | Target |
| 2-Methylphenanthrene | 192.25 | Target | Dibenzo[a,l]pyrene | 302.37 | Target |
| 2-Methylanthracene | 192.25 | Target | Naphtho[2,3-k]fluoranthene | 302.37 | Target |
| 1-Methylphenanthrene | 192.25 | Target | Naphtho[2,3-e]pyrene | 302.37 | Target |
| 9-Methylanthracene | 192.25 | Target | Dibenzo[a,e]pyrene | 302.37 | Target |
| 3,6-Dimethylphenanthrene | 206.28 | Target | Coronene | 300.35 | Target |
| 2,3-Dimethylanthracene | 206.28 | Target | Dibenzo[e,l]pyrene | 302.36 | Target |
| Fluoranthene | 202.26 | Target | Naphtho[2,3-a]pyrene | 302.36 | Target |
| 9,10-Dimethylanthracene | 206.28 | Target | Benzo[b]perylene | 302.36 | Target |
| Pyrene | 202.25 | Target | Dibenzo[a,i]pyrene | 302.36 | Target |
| Retene | 234.33 | Target | Benzo[ghi]perylene | 302.36 | Target |

**Table S2** PAH surrogates and target compounds in PUF and filter analysis method

| PAH | Molecular Weight ($g\ mol^{-1}$) | Target, Internal Standard (IS), or Surrogate |
|---|---|---|
| Naphthalene-d8 | 136.22 | IS |
| Acenaphthene-d10 | 160.25 | IS |
| Phenanthrene-d10 | 188.30 | IS |
| Chrysene-d12 | 240.36 | IS |
| Perylene-d12 | 264.34 | IS |
| 1-Methylnaphthalene-d10 | 152.26 | Surrogate |
| p-Terphenyl-d14 | 244.40 | Surrogate |
| Naphthalene | 128.17 | Target |
| 2-Methylnaphthalene | 142.20 | Target |
| 1-Methylnaphthalene | 142.20 | Target |
| Acenaphthylene | 152.19 | Target |
| Acenaphthene | 154.20 | Target |
| Fluorene | 166.22 | Target |
| Phenanthrene | 178.23 | Target |
| Anthracene | 178.23 | Target |
| 2-Methylphenanthrene | 192.25 | Target |
| 1-Methylphenanthrene | 192.25 | Target |
| Fluoranthene | 202.26 | Target |
| Pyrene | 202.25 | Target |
| Benz[a]anthracene | 228.29 | Target |
| Chrysene/Iso-chrysene | 228.28 | Target |
| Benzo[b]fluoranthene | 252.30 | Target |
| Benzo[k]fluoranthene | 252.30 | Target |
| Benzo[a]pyrene | 252.30 | Target |
| Indeno[1,2,3-c,d]pyrene | 276.33 | Target |
| Dibenzo[a,h]pyrene | 278.35 | Target |
| Benzo[ghi]perylene | 302.36 | Target |

**Table S3** Hydroxy-PAH target compounds and LODs in urine analysis method

| Target Hydroxy-PAH (OH-PAH) | Limit of Detection (LOD) ng/mL |
|---|---|
| 1-OH-naphthalene | 0.06 |
| 2-OH-naphthalene | 0.09 |
| 2-OH-fluorene | 0.008 |
| 3-OH-fluorene | 0.008 |
| 1-OH-phenanthrene | 0.009 |
| 2-OH- & 3-OH-phenanthrene | 0.01 |
| 4-OH-phenanthrene | 0.007 |
| 1-OH-pyrene | 0.07 |

**Table S4** Urinary OH-PAH metabolite ratios for naphthalene, fluorene, and phenanthrene. The metabolite with the lowest concentration has a value of one in each ratio

| Individual | 1-OH-naphthalene | : | 2-OH-naphthalene | 2-OH-fluorene | : | 3-OH-fluorene | 1-OH-phenanthrene | : | 2- & 3-OH-phenanthrene | : | 4-OH-phenanthrene |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1.0 | : | 3.6 | 4.1 | : | 1.0 | 7.2 | : | 3.3 | : | 1.0 |
| 2 | 1.0 | : | 12.8 | 5.1 | : | 1.0 | 1.3 | : | 2.7 | : | 1.0 |
| 3 | 1.0 | : | 5.0 | 3.2 | : | 1.0 | 5.1 | : | 3.8 | : | 1.0 |
| 4 | 1.0 | : | 1.2 | 2.0 | : | 1.0 | 7.0 | : | 4.3 | : | 1.0 |
| 5 | 1.0 | : | 3.2 | 3.1 | : | 1.0 | 4.3 | : | 4.2 | : | 1.0 |
| 6 | 1.0 | : | 2.4 | 3.1 | : | 1.0 | 4.6 | : | 4.1 | : | 1.0 |
| 7 | 1.0 | : | 5.3 | 4.0 | : | 1.0 | 6.6 | : | 3.7 | : | 1.0 |
| 8 | 1.0 | : | 12.9 | 2.5 | : | 1.0 | 2.2 | : | 3.3 | : | 1.0 |
| 9 | 1.0 | : | 66.9 | 1.9 | : | 1.0 | 1.2 | : | 1.9 | : | 1.0 |
| 10 | 1.0 | : | 9.9 | 5.8 | : | 1.0 | 1.7 | : | 3.4 | : | 1.0 |
| 11 | 1.0 | : | 8.5 | 3.8 | : | 1.0 | 5.4 | : | 3.3 | : | 1.0 |
| 12 | 1.0 | : | 4.9 | 2.8 | : | 1.0 | 6.1 | : | 2.4 | : | 1.0 |
| 13 | 1.0 | : | 19.8 | 4.0 | : | 1.0 | 5.0 | : | 3.5 | : | 1.0 |
| 14 | 1.0 | : | 3.0 | 5.0 | : | 1.0 | 2.8 | : | 2.6 | : | 1.0 |
| 15 | 1.0 | : | 1.7 | 3.6 | : | 1.0 | 7.6 | : | 3.7 | : | 1.0 |
| 16 | 1.0 | : | 6.4 | 4.7 | : | 1.0 | 7.6 | : | 3.4 | : | 1.0 |
| 17 | 1.0 | : | 4.1 | 3.2 | : | 1.0 | 3.2 | : | 3.4 | : | 1.0 |
| 18 | 1.0 | : | 5.1 | 2.2 | : | 1.0 | 3.3 | : | 2.9 | : | 1.0 |
| 19 | 1.0 | : | 21.0 | 4.2 | : | 1.0 | 1.8 | : | 3.0 | : | 1.0 |
| 20 | 1.0 | : | 2.3 | 4.5 | : | 1.0 | 6.4 | : | 3.1 | : | 1.0 |
| 21 | 1.0 | : | 6.8 | 5.1 | : | 1.0 | 9.4 | : | 6.0 | : | 1.0 |
| 22 | 1.0 | : | 17.0 | 4.2 | : | 1.0 | 6.7 | : | 3.2 | : | 1.0 |
| **Range** | 1.0 | : | 1.2 - 66.9 | 1.9 - 5.8 | : | 1.0 | 1.2 - 9.4 | : | 1.9 - 6.0 | : | 1.0 |
| **Average** | 1.0 | : | 10.18 | 3.7 | : | 1.0 | 4.8 | : | 3.4 | : | 1.0 |

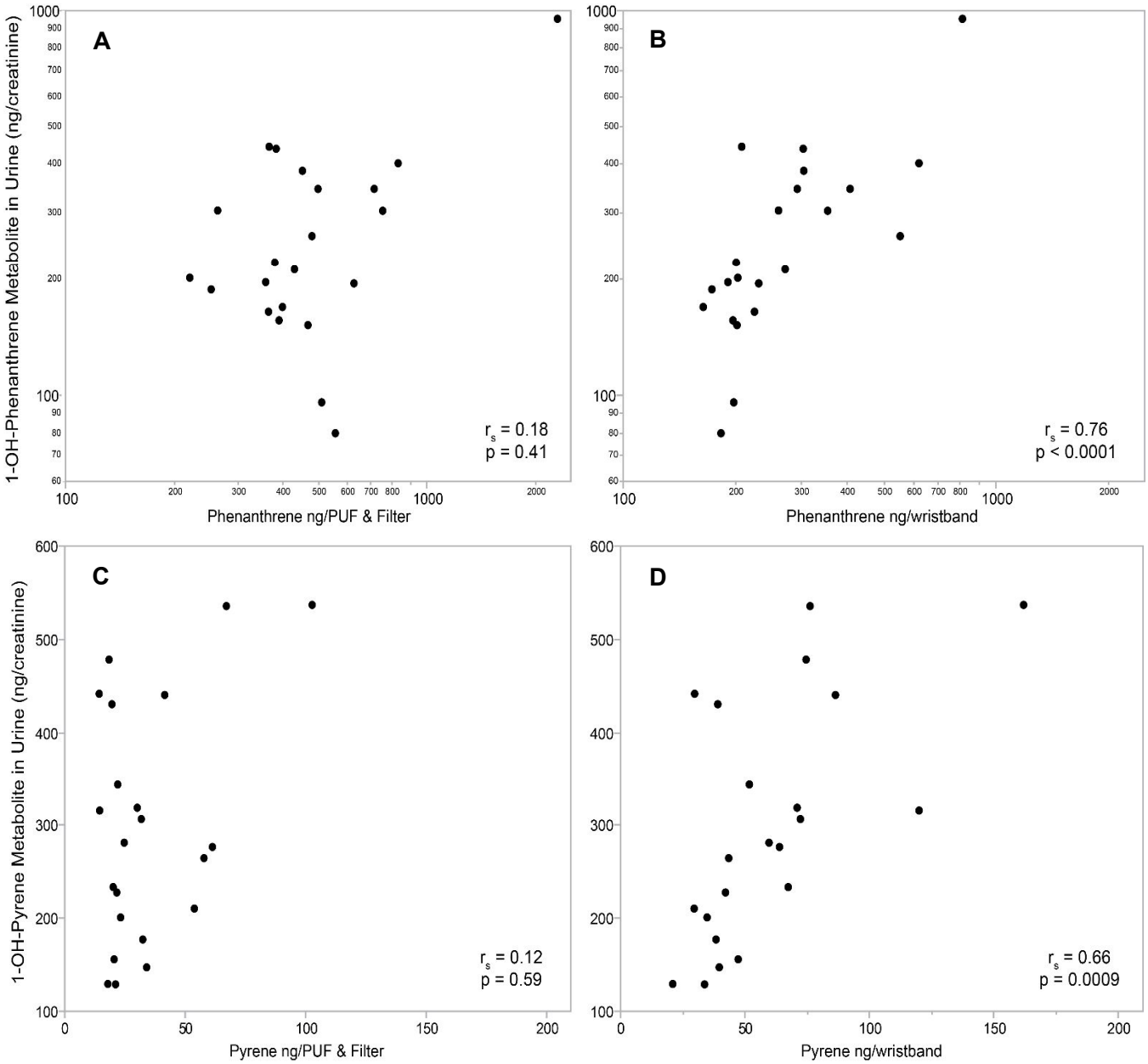


**Fig. S1** Phenanthrene correlation scatterplots for OH-PAH concentrations in urine and PAH concentrations in A) PUFs and filters and B) wristbands. Pyrene correlation scatterplots for OH-PAH concentrations in urine and PAH concentrations in C) PUFs and filters and D) wristbands