SUPPLEMENTAL INFORMATION

Assessing the external exposome using wearable passive samplers and high-resolution mass spectrometry among South African children participating in the VHEMBE study

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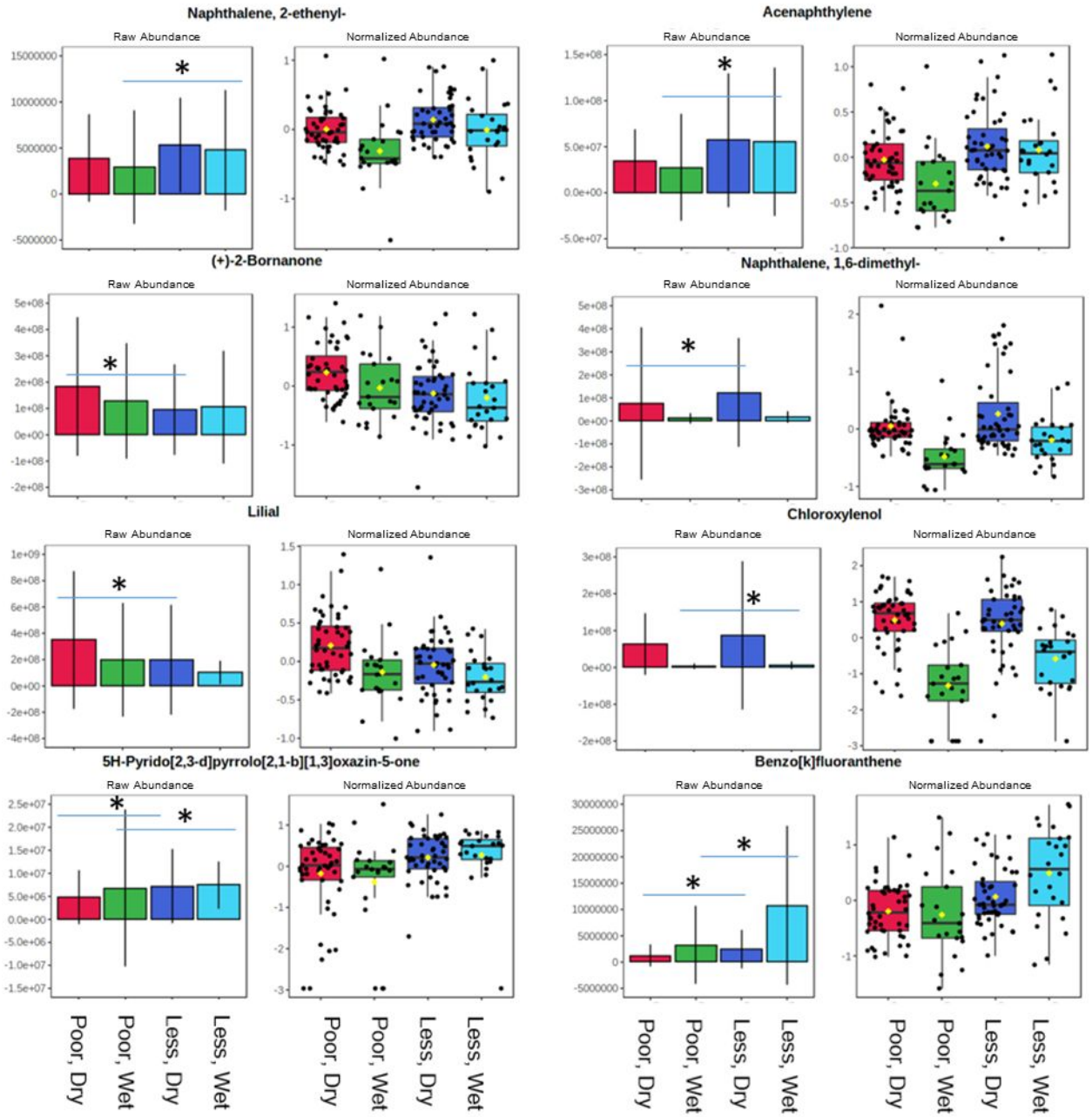
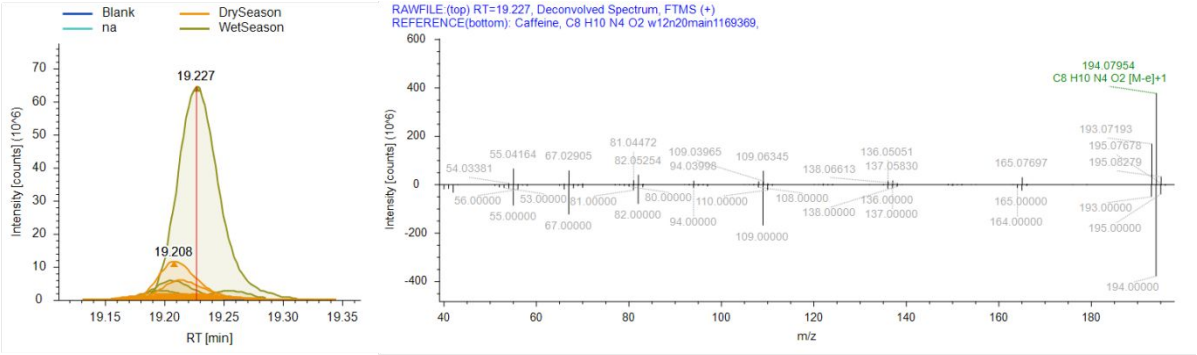


***Figure S1**: A subset of chemicals and their significance across poverty level (more poor: "poor", less poor: "less"), grouped by season (wet season: "wet", dry season: "dry"). Significance is based on a post-hoc Fisher's LSD test and ANOVA with Hochberg correction (adjusted p-value). Significant comparisons between poor and less poor are shown. Raw and normalized (log-scaled and mean centered) abundance data are shown, with statistics performed on the normalized data.*



Structure Name	Total Score	HRF Score	SI	ΔMass [ppm]	RI Delta
Caffeine	96.5	99.4	835	-1.46	8

Figure S2. *Spectral evidence used in suspect screening to identify caffeine. Note that a Level 2 (High Confidence) assignment was provided when RI delta < 50, RSI > 600, and RHRF > 75. In compounds of interest manual review was done to show that no other compounds in the library had a similar spectra and matching RI, and that other evidence including observation of molecular ion, isotopic ratios, peak shape, and database occurrence. For caffeine, all these lines of evidence were observed (molecular ion exact mass match, high EI and high-resolution mass filter score, retention index match, and quality peak shape higher than background signal). Given the caffeine is relative non-volatile, we expect the detected chemical was associated with deposited particulate. It is also useful to note the heterogeneity of exposures ranging across several magnitudes between participants.*