**NMR Metabolomics Methods for Cord Blood PAH Plasma Samples**

Aliquots of plasma samples (180 µL) were transferred into labeled tubes for experimental samples. Pooled male, female and combined plasma samples were prepared to serve as external QC samples. For all samples 20 µL of 10 mM formate solution (chemical shift indicator) in 0.9% saline with 0.02% NaN3 was added to each tube and were vortexed for 30 sec and centrifuged at 12000 rcf for 5 min. A 200 µL aliquot of the supernatant was transferred into 3 mm NMR tubes (Bruker-Biospin, Switzerland), which were kept on ice until data acquisition.

1H NMR spectra of plasma samples were acquired on a Bruker Avance III 700 MHz NMR spectrometer (located at the David H. Murdock Research Institute at Kannapolis, NC, USA) using a 5 mm cryogenically cooled ATMA inverse probe and ambient temperature of 25℃. A CPMG pulse sequence with presaturation (cpmgpr1d) was used for data acquisition. For each sample 512 transients were collected into 64k data points using a spectral width of 14.1 kHz (20.1 ppm), 2 s relaxation delay, 400 µs fixed echo time, loop for T2 filter (l4)=80, and an acquisition time of 2.324s per FID. The water resonance was suppressed using resonance irradiation during the relaxation delay. Spectra were zero filled, and Fourier transformed after exponential multiplication with line broadening factor of 0.5. Phase and baseline of the spectra were manually corrected for each spectrum. Spectra were referenced internally to the formate signal. The quality of each NMR spectrum was assessed for the level of noise and alignment of identified markers. Spectra were assessed for missing data and underwent quality checks.

NMR spectra were processed using ACD 1D NMR Processor 12.0 (ACD Labs, Toronto, CA). Spectra were zero filled, and Fourier transformed after exponential multiplication with line broadening factor of 0.5. Phase and baseline of the spectra were manually corrected for each spectrum. NMR bins (0.00-8.42 ppm) were made after excluding water (4.55-5.15 ppm) using intelligent binning width of 0.04 ppm and 50% looseness factor. Integrals of each of the bins were normalized to total integral of each of the spectrum.