

Weighted molar sums: inclusion and formulae

Individual compounds were included in groups if they were detected in $\geq 20\%$ of the samples, so as not to bias the resulting molar sums by including metabolite measures based on a preponderance of imputed data. Bisphenols that were detected in $\geq 50\%$ of the samples were analyzed separately. Because machine values were not available, bisphenol and phthalate metabolite concentrations below the level of detection (LOD) were substituted by $\text{LOD}/\sqrt{2}$, as routinely performed in bisphenol and phthalate analyses (Hornung and Reed, 1990).

Phthalic acid (PA) was used separately as a proxy of total phthalate exposure (Bang du, et al., 2011).

Formula for weighted molar sums in nmol per liter:

$((\text{concentration compound in ng/ml}) \times (1/\text{molecular weight in g/mol}) \times (1/10^{-3})) + ((\text{concentration compound in ng/ml}) \times (1/\text{molecular weight in g/mol}) \times (1/10^{-3})) + \text{etc.}$

Formula for creatinine adjusted compounds in μg per gram creatinine:

$((\text{concentration compound in ng/ml})/(\text{concentration urinary creatinine in } \mu\text{g/ml})) \times (1/10^{-3})$

Formula for creatinine adjusted weighted molar sums in μmol per gram creatinine:

$((\text{concentration in } \mu\text{g/g creatinine})/(\text{molecular weight in g/mol})) + ((\text{concentration in } \mu\text{g/g creatinine})/(\text{molecular weight in g/mol})) + \text{etc.}$

References

- Bang du Y, Lee IK, Lee BM. Toxicological characterization of phthalic Acid. *Toxicol Res* 2011;27:191–203.
- Hornung RW, Reed LD. Estimation of average concentration in the presence of non-detectable values. *Appl Occup Environ Hyg* 1990;5:46–51.