

Concentrations of phthalates and DINCH metabolites in pooled urine from Queensland, Australia

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Supplementary Material

Preparation of synthetic urine:

Analytical grade (>90%) sodium acetate, potassium chloride, sodium chloride, urea, citric acid, ascorbic acid, potassium phosphate, creatinine, sodium hydroxide, sodium bicarbonate and sulfuric acid were purchased from Sigma Aldrich (Sydney, Australia). Synthetic urine was prepared according to Calafat and Sampson (2009). Briefly, 3.8g potassium chloride, 8.5g sodium chloride, 24.5g urea, 1.03g citric acid, 0.34g ascorbic acid, 1.18g potassium phosphate, 1.4g creatinine, 0.64g sodium hydroxide, 0.47g sodium bicarbonate, and 0.28ml sulfuric acid were combined and diluted to 1L in a volumetric flask using ultrapure milli-Q water.

References:

Calafat AM, Sampson EJ (2009) Laboratory Procedure Manual: Bisphenol A and other environmental phenols and parabens in urine. Method number 6301.01. Available from: www.cdc.gov/nchs/data/nhanes. Date accessed: 9 July 2012

Table S1. Uses, exposure sources and main urinary biomarkers of phthalates and DINCH

Parent compound	General Uses	Specific Uses	Exposure sources
Low molecular weight phthalates			
Di-n-butyl phthalate (DnBP)	Used as solvents, adhesives, denaturants and fixatives in cosmetics and PCPs	PVC applications, adhesives and coatings. Medicaments, cosmetics, food packing, food.	Dermal exposure [1], diet [2], indoor dust [3] <i>Children</i> - indoor air/dust [1] <i>Adolescents and adults</i> - personal care products [1]
Diisobutyl phthalate (DiBP)		Food processing, equipment and food packing/ Cosmetics, food	Inhalation [3], diet [2] <i>Children</i> - dust [1]
Diethyl phthalate (DEP)		Plastics, fragrances, cosmetics, PCPs and medications/perfume, deodorant, lipstick, nail polish, body/face cream, after shave cream. Babies- lotion, shampoo, powder.	Dermal exposure [1], inhalation [3]
Dimethyl phthalate (DMP)		Solid propellants, plastics and insect repellents/Plastic bottles, food	Indoor air [3] <i>Adults</i> - personal care products [1]
High molecular weight phthalates			
Butyl benzyl phthalate (BBzP)		PVC flooring, paints, coatings, adhesives, printing inks, plastics. Food packing, food.	Diet [2], inhalation [3] <i>Infants and toddlers</i> -dust [1]; <i>Children</i> - diet [1] <i>Adults</i> - diet, spray paints [1]
Di(2-ethylhexyl) phthalate (DEHP)	Plasticizers in PVC material such as food packaging, flooring, and medical devices. In recent years, DINP and DIDP have increasingly replaced DEHP in these applications.	PVC applications, plastics, toys, cosmetics, medical equipment and tubing. Medical devices (bags for blood, parenteral nutrition, tubings and catheters). Food, food packing.	Diet [2], indoor dust [3] <i>Infants</i> - toys [1]
Diisononyl phthalate (DINP)		Alternative to DEHP in PVC manufacturing. PVC applications, toys, flooring, wall covering, inks, paints, and sealants.	Diet [2] <i>Children</i> , infants-mouthing of soft plastics [1] <i>Adults</i> - diet, dust, air, spray paints. [1]
Di-n-octyl phthalate (DnOP) & other HMW phthalates		PVC applications, food, food packing, Gloves and flooring	Diet [2]
Diisodecyl phthalate (DIDP)		Alternative to DEHP in PVC manufacturing. PVC applications, toys, wire and cables, flooring.	Diet [2] <i>Children, infants</i> - mouthing of soft plastics, dust, indoor air [1] <i>Adults</i> - diet, dust [1]
Other			
1,2-Cyclohexane dicarboxylic acid, diisononyl ester (DINCH)		Alternative to DEHP in PVC manufacturing. PVC applications, medical devices, toys, food packing.	Diet [2]

[1] Wormuth, M., Scheringer, M., Vollenweider, M., Hungerbühler, K. (2006). What are the sources of exposure to eight frequently used phthalic acid esters in Europeans? Risk Analysis. 26 (3), 803-824.

[2] Serrano SE, Braun J, Trasande L, Dills R, Sathyanarayana S. (2014) Phthalates and diet: a review of the food monitoring and epidemiology data. Environ Health. 13(1), 43.

[3] North ML, Takaro TK, Diamond ML, Ellis AK. Effects of phthalates on the development and expression of allergic disease and asthma. (2014) Ann. Allergy Asthma Immunol. 112(6), 496-502.

Table S2: Concentration (ng/mL) of free (% free) phthalate metabolite and DINCH species. Each pool represents 100 individuals.

Pool #	Sex	Age strata (years)	Av. Age (years)	MBP	MiBP	MEP	MMP	MBzP	MEHP	MEHHP	MEOHP	MECPP	MCOP	MNP	MCPP	MCNP	MHINCH
1	M	0-4	2.93	1.9(5)	2.1(6.3)	58.8(79)	6.5(100)	0.8(8.7)	0.6(5.8)	3.8(11)	2.4(9.3)	45.7(64)	21.4(74)	<LOD(N/A)	13.9(83)	1.7(57)	<LOD(N/A)
2	M		2.74	1.3(5.5)	1.2(5.7)	78.4(73)	1.4(100)	0.5(12)	<LOD(N/A)	1.8(11)	1.2(9.4)	18.9(53)	15.5(53)	<LOD(N/A)	3.1(67)	1.6(62)	<LOD(N/A)
3	F		3.33	2.3(6.2)	2.1(6.7)	56.2(79)	7.6(100)	0.6(9.8)	0.6(13)	1.8(7)	1.4(7.5)	28.2(52)	14(52)	<LOD(N/A)	2.9(67)	1.4(61)	<LOD(N/A)
4	F		3.24	1.5(6.5)	1.4(6.4)	23.2(79)	<LOD(N/A)	0.5(13)	<LOD(N/A)	2(8.7)	1.3(9)	23.2(54)	19.5(53)	<LOD(N/A)	3.6(82)	1.8(62)	<LOD(N/A)
5	M	5-14	8.83	3(7)	2.9(8.3)	33.5(71)	3.4(94)	1.3(13)	1(19)	2.7(8.7)	2.1(10)	28.5(52)	20.6(49)	<LOD(N/A)	4.3(81)	2(65)	<LOD(N/A)
6	M		9.21	1.3(6)	1.4(6)	72.4(85)	2(95)	0.5(9.6)	0.7(20)	1.7(7.7)	1.5(11)	20.4(51)	15.4(51)	<LOD(N/A)	2.6(74)	1.8(67)	<LOD(N/A)
7	F		8.74	3.6(12)	5.8(18)	66.8(70)	3.7(93)	0.8(15)	<LOD(N/A)	4(9.3)	2.5(10)	42.7(59)	19.3(61)	<LOD(N/A)	3.1(74)	2.3(72)	<LOD(N/A)
8	F		9.54	2.6(8.8)	1.6(5.2)	53.4(81)	2.8(140)	0.5(11)	<LOD(N/A)	1.9(8.1)	1.4(9.3)	22.5(51)	20.3(50)	<LOD(N/A)	4.5(76)	1.4(52)	<LOD(N/A)
9	M	15-29	24.28	0.5(2.4)	0.4(2.2)	59.1(74)	3.5(100)	0.4(9.1)	0.8(6.8)	2.8(6.8)	1.9(9.2)	29.1(44)	64.5(52)	1.3(10.6)	11.5(72)	3.8(62)	<LOD(N/A)
10	M		23.98	1.4(5.9)	0.8(3.7)	84.5(90)	2.6(100)	0.7(10)	<LOD(N/A)	2.8(6.9)	1.7(7.4)	26.3(50)	25.9(50)	<LOD(N/A)	5.8(76)	2.3(62)	<LOD(N/A)
11	F		24.05	1.2(3.9)	1.5(4.8)	129(71)	1.5(94)	0.6(7.7)	<LOD(N/A)	2.3(5.8)	1.9(7.9)	21.2(41)	21.5(41)	<LOD(N/A)	4.2(66)	1.8(50)	<LOD(N/A)
12	F		23.39	1.5(6.1)	1.3(6.4)	120(92)	<LOD(N/A)	0.5(9.6)	<LOD(N/A)	1.7(7.4)	1.4(9.9)	15.4(41)	22.5(48)	<LOD(N/A)	3.4(76)	1.5(56)	<LOD(N/A)
13	M	30-44	37.77	0.6(2.4)	0.6(2.5)	104(72)	1.4(93)	0.6(7.6)	0.5(4.2)	1.9(5.2)	1.5(7.2)	22.7(49)	24.6(45)	<LOD(N/A)	3.8(53)	1.6(50)	<LOD(N/A)
14	M		37.33	<LOD(N/A)	0.3(1.5)	202(81)	1.6(94)	0.5(7.5)	<LOD(N/A)	1.1(5.1)	1.1(8.3)	13.2(42)	17.5(38)	<LOD(N/A)	4.7(53)	1.1(46)	<LOD(N/A)
15	F		36.73	1(6)	1.1(7.1)	113(81)	7.3(100)	0.6(13)	<LOD(N/A)	1.9(9.5)	1.4(10)	16.8(44)	14.3(57)	<LOD(N/A)	2.7(66)	1.1(58)	<LOD(N/A)
16	F		36.78	0.7(3.5)	0.7(3.7)	81.2(77)	<LOD(N/A)	0.5(9.8)	0.6(12)	1.7(7)	1.3(7.6)	17.3(37)	27.4(47)	<LOD(N/A)	9.6(52)	1.9(58)	<LOD(N/A)
17	M	45-59	52.94	<LOD(N/A)	<LOD(N/A)	180(75)	1.7(81)	0.3(6.1)	<LOD(N/A)	1.3(6.1)	0.9(7.1)	12.2(42)	23(51)	<LOD(N/A)	4.1(64)	1.5(54)	<LOD(N/A)
18	M		53.15	0.4(1.5)	0.2(0.9)	96.2(68)	19.5(91)	0.4(6.9)	0.8(15)	1.8(6.1)	1.2(7.7)	17.9(42)	24.2(48)	<LOD(N/A)	3.1(50)	1.5(48)	<LOD(N/A)
19	F		53.29	2.5(5.6)	0.7(6.4)	664(86)	3.5(100)	0.3(9.7)	1.2(14)	2.6(7)	1.7(7.8)	26.2(52)	19(45)	0.5(7)	8.4(75)	1.5(58)	<LOD(N/A)
20	F		53.05	1(6.6)	1(7.2)	191(88)	<LOD(N/A)	0.4(13)	<LOD(N/A)	1.2(8.6)	0.9(11)	10.8(43)	18.7(55)	<LOD(N/A)	13.6(72)	1.2(57)	<LOD(N/A)
21	M	>60	73.71	<LOD(N/A)	<LOD(N/A)	138(57)	1.1(100)	0.3(7)	1.9(33)	1(5.5)	0.9(9.1)	11.1(40)	11.9(45)	<LOD(N/A)	2.2(56)	1.1(48)	<LOD(N/A)
22	M		71.91	1.3(3.6)	1.4(8.6)	65.1(61)	<LOD(N/A)	0.5(8.5)	0.8(14)	1.3(6.9)	1.2(11)	13.9(45)	12.7(48)	<LOD(N/A)	3(59)	1.1(55)	<LOD(N/A)
23	F		75.07	1.2(7.7)	1.7(9.6)	142(76)	<LOD(N/A)	0.5(15)	2.4(36)	2(10)	1.4(13)	12.3(44)	14.7(49)	<LOD(N/A)	2.1(55)	1.1(48)	0.5(3.8)
24	F		76.08	1(7.2)	0.8(5.4)	232(87)	<LOD(N/A)	0.4(13)	<LOD(N/A)	1.7(8.5)	1.1(11)	10.4(41)	12.5(46)	<LOD(N/A)	3.1(76)	1.4(58)	<LOD(N/A)

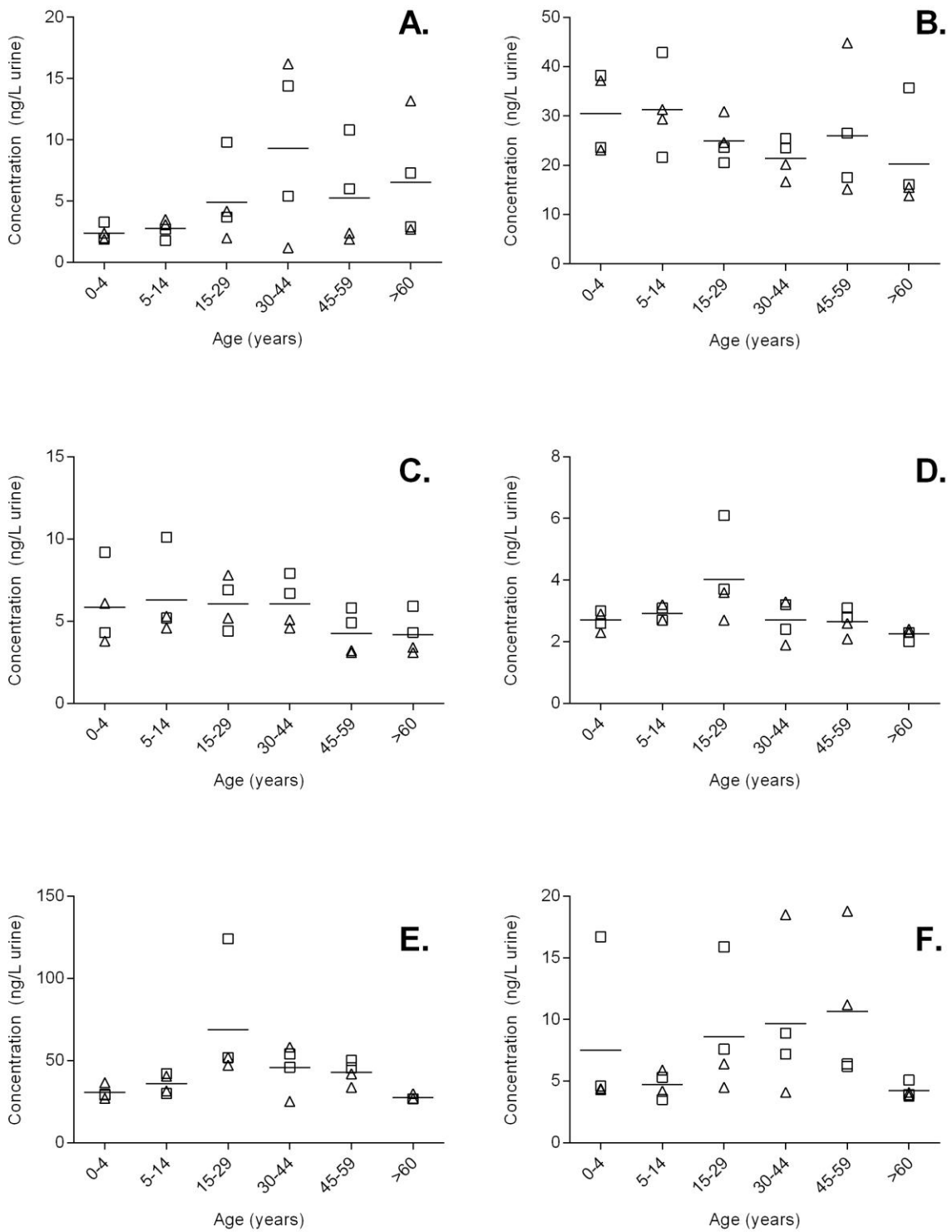


Figure S1: Urinary total concentration (ng/mL) versus age (years) for MHINCH (A), MBP (B), MBzP (C), MCNP (D), MCOP (E) and MCPP (F). Triangles denote female pools, squares denote male pools. Horizontal line indicates mean concentration of four pools in each age strata.

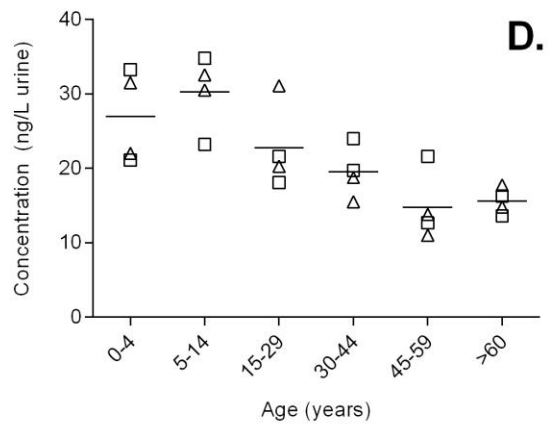
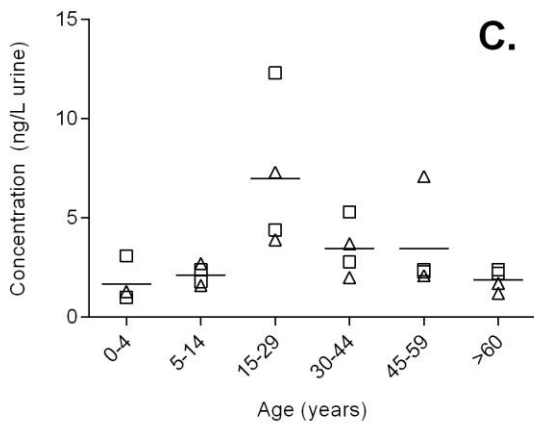
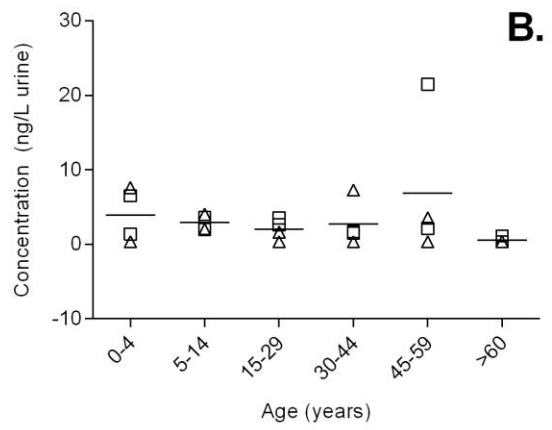
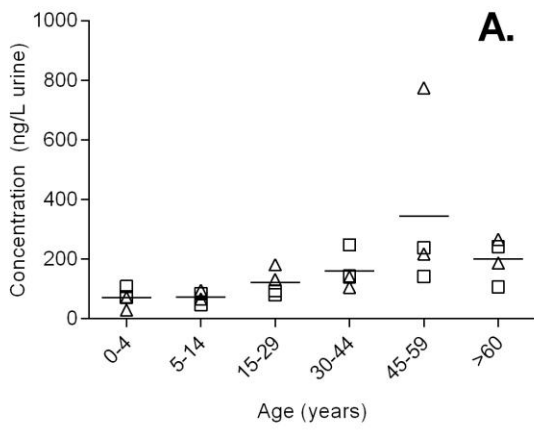


Figure S2: Urinary total concentration (ng/mL) versus age (years) for MEP (A), MMP (B), MNP (C) and MiBP (D). Triangles denote female pools, squares denote male pools. Horizontal line indicates mean concentration of four pools in each age strata.