

Analytical and Bioanalytical Chemistry

Electronic Supplementary Material

Development of urine standard reference materials for metabolites of organic chemicals including polycyclic aromatic hydrocarbons, phthalates, phenols, parabens, and volatile organic compounds

Michele M. Schantz, Bruce A. Benner, Jr., N. Alan Heckert, Lane C. Sander, Katherine E. Sharpless, Stacy S. Vander Pol, Y. Vasquez, M. Villegas, Stephen A. Wise, K. Udeni Alwis, Benjamin C. Blount, Antonia M. Calafat, Zheng Li, Manori J. Silva, Xiaoyun Ye, Éric Gaudreau, Donald G. Patterson, Jr, Andreas Sjödin

Table S1 Mass Fractions (ng/g) in SRM 3672

	NIST (n=20)		CDC (n=24)		INSPQ (n=4)	
	Mean	Std Dev	Mean	Std Dev	Mean	Std Dev
1-OH-naphthalene	33.7	1.1	37.4	2.0	29.8	2.2
2-OH-naphthalene	8.67	0.20	8.47	0.41	8.46	0.33
9-OH-fluorene	0.343	0.021	0.389	0.019	0.258	0.012
3-OH-fluorene	0.426	0.014	0.431	0.022	0.403	0.005
2-OH-fluorene	0.863	0.023	0.858	0.044	0.842	0.008
4-OH-phenanthrene	0.050	0.003	0.044	0.002	0.050	0.001
9-OH-phenanthrene	0.093	0.003	not reported		0.099	0.013
3-OH-phenanthrene	0.117	0.009	0.126	0.014	0.127	0.006
1-OH-phenanthrene	0.129	0.008	0.124	0.009	0.146	0.006
2-OH-phenanthrene	0.082	0.005	0.082	0.005	0.082	0.004
1-OH-pyrene	0.177	0.006	0.173	0.010	0.157	0.010

Table S2 Mass Fractions (ng/g) in SRM 3673

	NIST (n=20)		CDC (n=24)		INSPQ (n=4)	
	Mean	Std Dev	Mean	Std Dev	Mean	Std Dev
1-OH-naphthalene	210	8	233	16	174	14
2-OH-naphthalene	1.34	0.07	1.31	0.06	1.25	0.10
9-OH-fluorene	0.111	0.013	0.125	0.006	0.088	0.004
3-OH-fluorene	0.038	0.006	0.042	0.008	0.034	0.005
2-OH-fluorene	0.112	0.010	0.105	0.006	0.100	0.003
4-OH-phenanthrene	0.011	0.001	0.010	0.001	0.010	0.000
9-OH-phenanthrene	0.011	0.001	not reported		0.012	0.001
3-OH-phenanthrene	0.031	0.005	0.031	0.023	0.028	0.002
1-OH-phenanthrene	0.048	0.006	0.043	0.003	0.053	0.001
2-OH-phenanthrene	0.023	0.004	0.022	0.002	0.028	0.001
1-OH-pyrene	0.031	0.004	0.030	0.005	0.027	0.003