

Supporting Information for Quantification of Metabolites for Assessing Human Exposure to Soapberry Toxins Hypoglycin A and Methylenecyclopropylglycine

Samantha L. Isenberg;¹ Melissa D. Carter;^{2*} Leigh Ann Graham;¹ Thomas P. Mathews;¹ Darryl Johnson;¹ Jerry D. Thomas;² James L. Pirkle;² Rudolph C. Johnson²

¹Oak Ridge Institute for Science and Education Fellow at the Centers for Disease Control and Prevention, Atlanta, GA

²Division of Laboratory Sciences, National Center for Environmental Health, Centers for Disease Control and Prevention, Atlanta, GA

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Table S1. For evaluation of ion suppression, MCPF-Gly and MCPA-Gly calibrators were prepared in both urine and water, and the average peak areas (n = 4) from urine and water were used to calculate a % difference.

Analyte	Conc. (µg/mL)	Urine (n=4)	Water (n=4)	% Ion suppression ^a ± SD ^b
		mean pk area ± SD	mean pk area ± SD	
MCPF-Gly	0.200	$(2.49 \pm 0.20) \times 10^3$	$(2.36 \pm 0.30) \times 10^3$	105 ± 16 %
	1.00	$(1.06 \pm 0.04) \times 10^4$	$(1.04 \pm 0.05) \times 10^4$	102 ± 6 %
	5.00	$(5.11 \pm 0.42) \times 10^4$	$(4.88 \pm 0.06) \times 10^4$	105 ± 9 %
MCPA-Gly	0.200	$(6.10 \pm 0.87) \times 10^3$	$(5.76 \pm 0.21) \times 10^3$	106 ± 15 %
	1.00	$(2.79 \pm 0.05) \times 10^4$	$(2.72 \pm 0.16) \times 10^4$	102 ± 6 %
	5.00	$(1.34 \pm 0.08) \times 10^5$	$(1.30 \pm 0.02) \times 10^5$	103 ± 6 %

^a % Ion suppression = [(pk area for urine sample)/(pk area for water sample)] * 100

^b SD = % difference * [(SD of difference / difference)² + (SD of average / average)²]^{1/2}

Table S2. Post-preparative stability of QCs (n = 4) in a 5 °C autosampler evaluated at 0, 24, and 72 hours.

Analyte	QC	0 hours			24 hours			72 hours		
		conc	% RSD	% RE	conc	% RSD	% RE	conc	%RSD	% RE
MCPF-Gly	QH	7.19	6.3	2.6%	7.48	3.7	6.8%	7.51	3.5	7.3%
	QM	1.55	7.4	3.5%	1.53	5.6	1.7%	1.63	4.3	8.5%
	QL	0.274	10	-8.8%	0.285	8.6	-5.1%	0.289	11	-3.8%
MCPA-Gly	QH	7.23	2.4	3.3%	7.34	2.5	4.9%	7.21	2.9	2.9%
	QM	1.51	8.5	0.5%	1.53	2.7	1.8%	1.56	5.0	4.0%
	QL	0.269	15	-10%	0.283	1.2	-5.8%	0.292	6.0	-2.7%