**Supporting Information for**

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

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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 suppressiona** **±** **SDb** |
| **mean pk area ± SD** | **mean pk area** ± **SD** |
|  | **0.200** | (2.49 ± 0.20) × 103 | (2.36 ± 0.30) × 103 | 105 ± 16 % |
| **MCPF-Gly** | **1.00** | (1.06 ± 0.04) × 104 | (1.04 ± 0.05) × 104 | 102 ± 6 % |
|  | **5.00** | (5.11 ± 0.42) × 104 | (4.88 ± 0.06) × 104 | 105 ± 9 % |
|  | **0.200** | (6.10 ± 0.87) × 103 | (5.76 ± 0.21) × 103 | 106 ± 15 % |
| **MCPA-Gly** | **1.00** | (2.79 ± 0.05) × 104 | (2.72 ± 0.16) × 104 | 102 ± 6 % |
|  | **5.00** | (1.34 ± 0.08) × 105 | (1.30 ± 0.02) × 105 | 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* |
|  | *QH* |  | 7.19 | 6.3 | 2.6% |  | 7.48 | 3.7 | 6.8% |  | 7.51 | 3.5 | 7.3% |
| **MCPF-Gly** | *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% |
|  | *QH* |  | 7.23 | 2.4 | 3.3% |  | 7.34 | 2.5 | 4.9% |  | 7.21 | 2.9 | 2.9% |
| **MCPA-Gly** | *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% |