

Supplementary Materials: Toxicokinetic Properties of Glyphosate, a Vehicle-Dependent Herbicide, in Rats

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Table S1. Analytical LC condition of glyphosate and AMPA.

| Instrument | | |
|------------------------------|---|----|
| HPLC | Agilent Infinity 1290 LC | |
| Column | Hypercarb column (100 × 2.1 mm, 5 μm) | |
| Guard column | Security Guard Cartridges RP-1 (4 × 3.0 mm) | |
| LC condition | | |
| Mobile Phase | A: 5 mM ammonium acetate in DW (1% formic acid) | |
| | B: ACN (1% formic acid) | |
| Column oven temperature (°C) | 25 | |
| Autosampler temperature (°C) | 4 | |
| Flow rate (mL/min) | 0.3 | |
| Running time (min) | 10 | |
| Injection volume (μl) | 10 | |
| Gradient condition | | |
| Time (min) | A | B |
| 0 | 80 | 20 |
| 2.5 | 80 | 20 |
| 6 | 20 | 80 |
| 8 | 20 | 80 |
| 9 | 80 | 20 |
| 10 | 80 | 20 |

Table S2. Optimized MS/MS parameters of glyphosate, AMPA and 4-hydroxyacetanilide (IS) and analytical MS/MS condition.

| Compound | ESI mode | Precursor ion (m/z) | Product ion (m/z) | CE * (V) | DP ** (V) |
|---------------------------|----------|-------------------------------------|----------------------|----------|-----------|
| Glyphosate | Negative | 168 | 62.8 | -30 | -55 |
| | | 168 | 78.8 | -60 | |
| AMPA | Negative | 109.9 | 63 | -24 | -25 |
| | | 109.9 | 78.8 | -38 | |
| 4-hydroxyacetanilide (IS) | Positive | 152.1 | 110.2 | 23 | 41 |
| MS/MS Instrument | | AB SCIEX API 4000 | | | |
| MS/MS condition | | | | | |
| Curtain gas (L/min) | | | 20 | | |
| Ion spray voltage (V) | | - 4200 (negative) / 4200 (positive) | | | |
| Ion source gas 1 (L/min) | | | 50 | | |
| Ion source gas 2 (L/min) | | | 55 | | |
| Source temperature (°C) | | | 550 | | |

CE *: Collision energy; DP **: Declustering potential

Table S3. Accuracy, precision and linearity at LLOQ of glyphosate and AMPA (0.5 µg/mL) (n=5).

| n | Concentration (µg/mL) | Glyphosate | AMPA |
|--|-----------------------|-------------|-------------|
| 1 | 0.5 | 0.50 | 0.41 |
| 2 | | 0.59 | 0.48 |
| 3 | | 0.58 | 0.59 |
| 4 | | 0.60 | 0.59 |
| 5 | | 0.58 | 0.57 |
| Mean ± SD | | 0.57 ± 0.04 | 0.53 ± 0.08 |
| Accuracy (%) ¹ | | 113.40 | 105.20 |
| Precision (%) ² | | 7.00 | 14.90 |
| Linearity (r ²) ³ | | 0.9995 | 0.9996 |

Accuracy (%)¹ (measured concentration/nominal concentration) × 100; Precision (%)² (standard deviation / mean) × 100; Linearity (r²)³ correlation coefficient

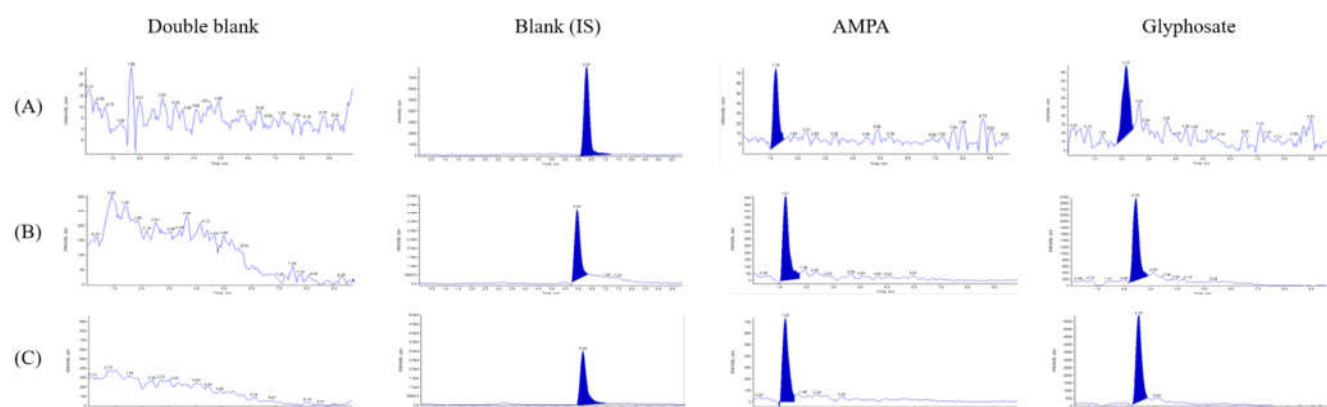


Figure S1. Representative MRM chromatograms of glyphosate, AMPA and 4-hydroxyacetanilide (internal standard, IS) obtained at LLOQ (0.5 $\mu\text{g/mL}$) in plasma (A), liver (B) and kidney (C).