Table S1. Summary of the MS\(^2\) data for prometryn and its metabolites in root exudates from celery under hydroponic cultivation

| Analyte                   | Retention time (min) | Theoretical m/z, [M+H]\(^+\) | Experimental m/z, [M+H]\(^+\) | Delta ppm | MS\(^2\) fragments                  |
|---------------------------|----------------------|-------------------------------|-------------------------------|-----------|-------------------------------------|
| Prometryn                 | 8.37                 | 242.1434                      | 242.1428                      | 2.48      | 200.0961, 158.0493                  |
| Deethy lametryn           | 5.19                 | 200.0964                      | 200.0960                      | −2.00     | 158.0492                            |
| Hydroxypropazine          | 4.94                 | 212.1506                      | 212.1502                      | −1.89     | 170.1033, 128.0566, 240.1292,       |
| Prometryn sulfoxide       | 7.43                 | 258.1383                      | 258.1373                      | −3.87     | 212.1500, 128.0823, 212.1501,       |
| Prometryn sulfone         | 8.14                 | 274.1332                      | 274.1324                      | −2.92     | 170.1033, 128.0563, 86.0353         |
| Didealkylametryn          | 1.41                 | 158.0495                      | 158.0492                      | −1.90     | 158.0492, 110.0463                  |
| Hydroxydeethylatrazine    | 1.11                 | 170.1036                      | 170.1033                      | −1.76     | 128.0566, 86.0354                   |
Table S2. Summary of linearity, limit of detection (LOD), limit of quantification (LOQ), recovery, and precision data for target compounds

| Analyte               | Linearity range | $R^2$ | LOD (μg/L) | LOQ (μg/L) | Spiked levels (μg/L) | Mean recoveries, % (precision, %, $n = 6$) |
|-----------------------|-----------------|------|-------------|-------------|----------------------|-------------------------------------------|
| Prometryn            | 1.0–200         | 0.997| 0.01        | 0.03        | 10, 50, 100          | 107.9 (9.6), 104.9 (6.1), 102.4 (3.6)       |
| Deethylametryn       | 0.1–20          | 0.999| 0.04        | 0.12        | 1.0, 5.0, 10.0       | 83.4 (8.9), 88.0 (5.3), 96.1 (8.8)         |
| Hydroxypropazine     | 0.1–20          | 0.995| 0.04        | 0.12        | 1.0, 5.0, 10.0       | 84.4 (9.2), 92.0 (5.6), 100.4 (6.5)        |
| Prometryn sulfoxide  | 0.1–20          | 0.994| 0.02        | 0.06        | 1.0, 5.0, 10.0       | 95.9 (12.3), 108.6 (4.4), 102.7 (7.3)      |
| Prometryn sulfone    | 0.1–20          | 0.998| 0.04        | 0.12        | 1.0, 5.0, 10.0       | 78.0 (10.6), 82.0 (5.0), 83.8 (2.7)        |
| Didealkylametryn     | 0.1–20          | 0.994| 0.10        | 0.30        | 1.0, 5.0, 10.0       | 106.9 (13.0), 83.5 (10.8), 91.9 (6.7)      |
| Hydroxydeethylatrazi | 0.1–20          | 0.995| 0.10        | 0.30        | 1.0, 5.0, 10.0       | 80.6 (16.1),                               |
| ne  | 6   | 81.0 (18.2), |
|-----|-----|-------------|
|     |     | 83.4 (15.9) |