Supporting information for

**Identification of Dimethachlon Metabolites and** **Dissipation Behavior, Processing Factor and Risk Assessment of** **Dimethachlon in Rapeseed**

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**Table S1** **Instrumental Conditions for Metabolite Screening**

|  |  |  |
| --- | --- | --- |
| **Configuration** | **Item** | **Condition** |
| HPLCparameters | Chromatographic column | Accucore aQ column C18(150 mm × 2.1 mm; 2.6 μm) |
| Mobile phase(A: water, B: methanol) | time (min)05121414.116 | A (%)9898229898 | B (%)22989822 |
| Flow | 0.3 mL/min |
| Injection volume | 5 *µ*L |
| Column temperature | 40 °C |
| Sample temperature | 20 °C |
| HRMSParameters(ESI) | Scan mode | Full MS-dd/MS2 |
| Scan range | 70-1050 m/z |
| Resolution | 60000 |
| S-Lens RF Level | 70 |
| Sheath gas flow rate | 40 Arb |
| Aux gas flow rate | 10 Arb |
| heater temperature | 350℃ |
| capillary temperature | 320℃ |
| spray voltage (+) | 3500 V |
| Spray voltage (-) | -2500 V |
| AGC target for full mass | 3 × 106 |
| Maximum IT for full mass | 100 ms |
| Resolution for dd-MS2 | 15000 |
| AGC target for dd-MS2 | 1 × 105 |
| Maximum IT for dd-MS2 | 50 ms |
| Loop count | 5 |
| MSX count | 1 |
| Isolation window | 1.5 |
| Normalized collision energy | 20,40,60 (eV) |

**Table S2** **Instrument conditions for quantitative analysis of dimethachlon, DCBAA and 3,5-DCA**

|  |  |  |
| --- | --- | --- |
| **Configuration** | **Item** | **Condition** |
| HPLCparameters | Chromatographic column | Hypersil GOLD ™ C18(100 mm × 2.1 mm; 1.9 μm) |
| Mobile phase(A: water, B: acetonitrile) | time (min)6 | A (%)50 | B (%)50 |
| Flow | 0.2 mL/min |
| Injection volume | 5 µL |
| Column temperature | 40 °C |
| Sample temperature | 20 °C |
| HRMSParameters(APCI) | Scan mode | T-sim |
| Scan range | 70-1050 m/z |
| Resolution | 70000 |
| S-Lens RF Level | 50 |
| Sheath gas flow rate | 30 Arb |
| Aux gas flow rate | 5 Arb |
| heater temperature | 300 ℃ |
| capillary temperature | 320 ℃ |
| spray voltage (+) | 2.5μA |
| Spray voltage (-) | -2.5μA |



**Figure S1 The structure of** **dimethachlon**



**Figure S2 The** **structures of dimethachlon metabolites produced in mammals**



**Figure S3 The temperature during field experiments in Guiyang (April 18 to May 9, 2022) and Changsha (April 26 to May 17, 2022)**



Figure S 4. The HPLC-HRMS chromatograms of three target analytes on a Hypersil GOLD ™ C18 column with different mobile phase

(flow rate: 0.2 mL/min; injection volume: 5μL; solvent standard solution: 1 μg/mL)

1. acetonitrile : water = 70:30
2. acetonitrile : 0.1% formic acid water = 70:30
3. acetonitrile : water = 50:50

Figure S5. HPLC-HRMS chromatograms of three target analytes with different ion sources

(acetonitrile : water = 50:50; flow rate: 0.2 mL/min; injection volume: 5μL; solvent standard solution: 1 μg/mL, column: Hypersil GOLD ™ C18 )