

Supplementary for: Impact of matrix species and mass spectrometries on matrix effects in multi-residue pesticide analysis based on QuEChERS-LC-MS

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Table S1. Chemical abstracts service number (CAS No.), chemical classes, usage types, Octanol-water partition coefficient (K_{ow}), retention time (t_R , min), and adduct as well as theoretical m/z of precursor ions for 73 pesticides.

| Name | CAS No. | Chemical classes | Usage types | K_{ow} | t_R (min) | Adduct | Theoretical m/z |
|---------------------|-------------|------------------|---|----------|-------------|-----------|-----------------|
| Alachlor | 15972-60-8 | Chloroacetamide | Herbicide | 3.09 | 9.45 | $[M+H]^+$ | 270.1255 |
| Ametryn | 834-12-8 | Triazine | Herbicide | 2.63 | 6.81 | $[M+H]^+$ | 228.1277 |
| Atrazine | 1912-24-9 | Triazine | Herbicide | 2.7 | 7.61 | $[M+H]^+$ | 216.1011 |
| Carbendazim | 10605-21-7 | Benzimidazole | Fungicide, Metabolite | 1.48 | 4.02 | $[M+H]^+$ | 192.0768 |
| Chlordimeform | 6164-98-3 | Formamidine | Acaricide, Insecticide, Ovicide | 2.89 | 4.87 | $[M+H]^+$ | 197.0804 |
| Chlorpyrifos | 2921-88-2 | Organophosphate | Insecticide | 4.7 | 11.16 | $[M+H]^+$ | 321.9023 |
| Chlorpyrifos-methyl | 5598-13-0 | Organophosphate | Insecticide, Acaricide | 4 | 8.56 | $[M+H]^+$ | 349.9336 |
| Chlorsulfuron | 64902-72-3 | Sulfonylurea | Herbicide | 2.14 | 7.33 | $[M+H]^+$ | 358.0371 |
| Coumaphos10. | 56-72-4 | Organophosphate | Insecticide | 3.89 | 10.1 | $[M+H]^+$ | 363.0217 |
| Cyflufenamid | 180409-60-3 | Amidoxine | Fungicide | 4.7 | 10.36 | $[M+H]^+$ | 413.1283 |
| DEET | 134-62-3 | Unclassified | Insecticide, Repellent | 2.18 | 7.7 | $[M+H]^+$ | 192.1383 |
| Diazinon | 333-41-5 | Organophosphate | Insecticide, Acaricide, Repellent, Veterinary substance | 3.69 | 10.19 | $[M+H]^+$ | 305.1083 |
| Dichlorvos | 62-73-7 | Organophosphate | Insecticide, Acaricide | 1.9 | 6.87 | $[M+H]^+$ | 220.9532 |
| Diethofencarb | 87130-20-9 | Carbamate | Fungicide | 2.89 | 8.64 | $[M+H]^+$ | 268.1543 |
| Difenoconazole | 119446-68-3 | Triazole | Fungicide | 4.36 | 9.76 | $[M+H]^+$ | 406.0720 |
| Dimethenamid | 87674-68-8 | Chloroacetamide | Herbicide | 2.2 | 8.79 | $[M+H]^+$ | 276.0820 |
| Dimethoate | 60-51-5 | Organophosphate | Insecticide, Acaricide, Metabolite | 0.75 | 5.72 | $[M+H]^+$ | 230.0069 |
| Disulfoton | 298-04-4 | Organophosphate | Insecticide, Acaricide | 3.95 | 7.3 | / | / |

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|-----------------|-------------|-------------------------------|---|------|-------|--------------------|----------|
| Edifenphos | 17109-49-8 | Organophosphate | Fungicide | 3.83 | 9.65 | [M+H] ⁺ | 311.0324 |
| Epoxiconazole | 135319-73-2 | Triazole | Fungicide | 3.3 | 8.84 | [M+H] ⁺ | 330.0804 |
| Ethiofencarb | 29973-13-5 | Carbamate | Insecticide | 2.04 | 7.67 | [M+H] ⁺ | 226.0896 |
| Ethoprophos | 13194-48-4 | Organophosphate | Insecticide , Nematicide | 2.99 | 9.04 | [M+H] ⁺ | 243.0637 |
| Ethion | 563-12-2 | Organophosphate | Insecticide , Acaricide, Metabolite | 5.07 | 10.28 | [M+H] ⁺ | 384.9949 |
| Fenarimol | 60168-88-9 | Pyrimidine | Fungicide | 3.69 | 8.7 | [M+H] ⁺ | 331.0399 |
| Fenchlorphos | 299-84-3 | Organophosphate | Insecticide , Veterinary substance | 4.88 | 8.56 | [M+H] ⁺ | 320.9070 |
| Fenitrothion | 2255-17-6 | Organophosphate | Insecticide | 3.24 | 8.8 | / | / |
| Fenobucarb | 3766-81-2 | Carbamate | Insecticide | 2.78 | 8.5 | / | / |
| Fenpropathrin | 39515-41-8 | Pyrethroid | Insecticide , Acaricide | 6.04 | 11.19 | [M+H] ⁺ | 350.1751 |
| Fenthion | 55-38-9 | Organophosphate | Insecticide , Veterinary substance, Avicide | 4.84 | 9.9 | [M+H] ⁺ | 279.0273 |
| Fluazifop-butyl | 69806-50-4 | Aryloxyphenoxy pr-opionate | Herbicide | 4.5 | 9.34 | [M+H] ⁺ | 384.1417 |
| Fludioxonil | 131341-86-1 | Phenylpyrrole | Fungicide | 4.12 | 8.5 | [M+H] ⁺ | 249.0470 |
| Fluquinconazole | 136426-54-5 | Triazole | Fungicide | 3.24 | 8.96 | [M+H] ⁺ | 376.0163 |
| Flutriafol | 76674-21-0 | Triazole | Fungicide | 2.31 | 7.41 | [M+H] ⁺ | 302.1099 |
| Hexythiazox | 78587-05-0 | Carboxamide | Acaricide | 2.67 | 11.21 | [M+H] ⁺ | 353.1085 |
| Iprobenfos | 26087-47-8 | Organophosphate | Fungicide | 3.37 | 7.62 | [M+H] ⁺ | 289.1022 |
| Isazofos | 42509-80-8 | Organophosphate | Insecticide , Nematicide | 3.1 | 9.28 | [M+H] ⁺ | 314.0490 |
| Isoprocarb | 2631-40-5 | Carbamate | Insecticide | 2.32 | 9.28 | [M+H] ⁺ | 194.1176 |

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|------------------------|------------|-----------------|---|-------|-------|--------------------|----------|
| Malathion | 121-75-5 | Organophosphate | Insecticide , Acaricide, Veterinary substance | 2.75 | 9.25 | [M+H] ⁺ | 331.0433 |
| Metalaxyl | 57837-19-1 | Phenylamide | Fungicide | 1.75 | 7.71 | [M+H] ⁺ | 280.1543 |
| Methamidophos | 10265-92-6 | Organophosphate | Insecticide , Acaricide Metabolite | -0.82 | 1.06 | [M+H] ⁺ | 142.0086 |
| Methiathion | 950-37-8 | Organophosphate | Insecticide , Acaricide | 2.57 | 8.54 | [M+H] ⁺ | 302.9691 |
| Methyl-Parathion | 298-00-0 | Organophosphate | Insecticide | 3 | 8.93 | [M+H] ⁺ | 264.0090 |
| Metolachlor | 51218-45-2 | Chloroacetamide | Herbicide | 3.4 | 9.44 | / | / |
| Monocrotophos | 6923-22-4 | Organophosphate | Insecticide , Acaricide | 1.45 | 4.53 | [M+H] ⁺ | 224.0682 |
| Myclobutanil | 88671-89-0 | Triazole | Fungicide | 2.89 | 8.73 | [M+H] ⁺ | 289.1215 |
| Omethoate | 1113-02-6 | Organophosphate | Insecticide , Acaricide, Metabolite | -0.74 | 3.56 | [M+H] ⁺ | 214.0297 |
| Oxadixyl | 77732-09-3 | Phenylamide | Fungicide | 0.65 | 6.71 | [M+H] ⁺ | 279.1339 |
| Parathion | 56-38-2 | Organophosphate | Insecticide , Acaricide | 3.83 | 9.86 | [M+H] ⁺ | 292.0403 |
| Pendimethalin | 40487-42-1 | Dinitroaniline | Herbicide | 5.4 | 11.21 | [M+H] ⁺ | 282.1448 |
| Phorate | 298-02-2 | Organophosphate | Insecticide , Acaricide, Nematicide | 3.86 | 10.31 | / | / |
| Phorate sulfone | 251386 | Organophosphate | Insecticide , Metabolite | 4.14 | 8.38 | / | / |
| Phorate-oxon sulfoxide | 251417 | Organophosphate | Insecticide , Metabolite | 3.49 | 7.45 | / | / |
| Phosalone | 2310-17-0 | Organophosphate | Insecticide , Acaricide | 4.01 | 10.27 | [M+H] ⁺ | 367.9941 |
| Phosmet | 732-11-6 | Organophosphate | Insecticide , Acaricide, | 2.8 | 8.7 | [M+H] ⁺ | 318.0018 |

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|--------------------|-------------|-------------------|---|------|-------|--------------------|----------|
| | | | Veterinary substance | | | | |
| Phosphamidon | 13171-21-6 | Organophosphate | Insecticide , Acaricide | 0.8 | 6.45 | [M+H] ⁺ | 300.0762 |
| Piperonyl butoxide | 18693 | Cyclic aromatic | Veterinary substance | 4.75 | 10.88 | [M+H] ⁺ | 334.1349 |
| Pirimiphos methyl | 29232-93-7 | Organophosphate | Insecticide , Acaricide | 4.2 | 10.27 | [M+H] ⁺ | 306.1036 |
| Profenofos | 41198-08-7 | Organophosphate | Insecticide , Acaricide | 1.7 | 10.56 | [M+H] ⁺ | 372.9424 |
| Prometryn | 7287-19-6 | Triazine | Herbicide | 3.34 | 7.61 | [M+H] ⁺ | 242.1434 |
| Propargite | 2312-35-8 | Sulphite ester | Acaricide | 5.7 | 11.4 | / | / |
| Propazine | 139-40-2 | Triazine | Herbicide | 3.95 | 8.35 | [M+H] ⁺ | 230.1167 |
| Prothiofos | 34643-46-4 | Organophosphate | Insecticide | 5.67 | 11.94 | [M+H] ⁺ | 344.9701 |
| Pyridaben | 96489-71-3 | Pyridazinone | Insecticide , Acaricide | 6.37 | 11.75 | [M+H] ⁺ | 365.1449 |
| Pyridaphenthion | 119-12-0 | Organophosphate | Insecticide | 3.2 | 8.93 | [M+H] ⁺ | 341.0719 |
| Pyrimethanil | 53112-28-0 | Anilinopyrimidine | Fungicide | 2.84 | 7.45 | [M+H] ⁺ | 200.1182 |
| Pyroquilon | 57369-32-1 | Unclassified | Fungicide | 1.57 | 6.33 | [M+H] ⁺ | 174.0913 |
| Quinalphos | 13593-03-8 | Organophosphate | Insecticide , Acaricide | 4.44 | 9.79 | [M+H] ⁺ | 299.0614 |
| Tolclofos methyl | 57018-04-9 | Chlorophenyl | Fungicide | 3.8 | 6.42 | / | / |
| Tau-Fluvalinate | 102851-06-9 | Pyrethroid | Insecticide , Veterinary substance, Acaricide | 7.02 | 11.98 | [M+H] ⁺ | 503.1344 |
| Triadimenol | 55219-65-3 | Triazole | Fungicide, Metabolite | 3.18 | 8.3 | / | / |
| Triazophos | 24017-47-8 | Organophosphate | Insecticide , Acaricide, Nematicide | 3.55 | 9.27 | [M+H] ⁺ | 314.0723 |
| Triticonazole | 131983-72-7 | Triazole | Fungicide | 3.29 | 8.5 | / | / |
| Vamidothion | 2275-23-2 | Organophosphate | Insecticide , Acaricide | 0.15 | 5.21 | [M+H] ⁺ | 288.0488 |

Table S2 Latin plant names, botanical classifications, categories in the GB 23200.121-2021 National Food Safety Standard, categories in the Document N° SANTE/11312/2021, and code information in mass-spectrometry-related and chromatography-related comparisons of 32 commodities.

| Name | Latin name | Family | Categories in the GB 2763-2021 National Food Safety Standard | Categories in the Document N° SANTE/11312/2021 | Codes in mass-spectrometry-related comparisons |
|-----------------------|---|---------------|---|---|--|
| Cabbage | <i>Brassica oleracea</i> L. | Brassicaceae | Vegetables- Brassica class- Ball brassical | High water content-Brassica vegetables | IDA8 MRM8 |
| Mint | <i>Mentha haplocalyx</i> Briq. | Lamiaceae | Condiment-Leaf | High water content-Leafy vegetables and fresh herbs | IDA20 MRM20 |
| Wheatgrass | <i>Agropyron cristatum</i> (L.) Gaertn. | Poaceae | Vegetable-Leaf Vegetable- Green leafy vegetables | High water content-Leafy vegetables and fresh herbs | IDA30 MRM30 |
| <i>Amomum tsao-ko</i> | <i>Amomum tsaoko</i> Crevost et Lemarie | Zingiberaceae | Condiment-Fruits | High water content- Stem and stalk vegetables | IDA2 MRM2 |
| Orange | <i>Citrus sinensis</i> (L.) Osbeck | Rutaceae | Fruits-Citurs | High acid content and high water content-Citrus fruit | IDA22 MRM22 |
| Soybean | <i>Glycine max</i> (Linn.) Merr. | Fabaceae | Oil and grease- Large-scale oil seeds class | High oil content and very low water content-Oil seeds | IDA29 MRM29 |
| Red chili | <i>Capsicum annuum</i> L. | Solanaceae | Vegetable- Solanaceous Vegetable- Other Solanaceous Vegetable | High water content-fruiting vegetables/cucurbits | IDA25 MRM25 |

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|------------------------------|--|---------------------|---|---|----------------|
| Amaranth | <i>Amaranthus tricolor</i> L. | Amaranthaceae | Vegetable-Leaf Vegetable- Green leafy vegetables | High water content-Leafy vegetables and fresh herbs | IDA1 MRM1 |
| Sichuan pepper | <i>Zanthoxylum bungeanum</i> Maxim | Rutaceae | Condiment-Fruits | / | IDA28 MRM28 |
| Cowpea | <i>Vigna unguiculata</i> (Linn.) Walp. | Fabaceae | Vegetable-Legume- Pod edible legume | High water content-Fresh legume vegetables | IDA11 MRM11 |
| Blueberry | <i>Vaccinium Spp.</i> | <i>Ericaceae</i> | Fruits- berries and other small fruit- bind and shrubs | High acid content and high water content-Small fruit and berries | IDA7 MRM7 |
| Winged bean | <i>Psophocarpus tetragonolobus</i> (Linn.) D.C. | <i>Fabaceae</i> | Vegetable- Legume - Pod edible legume | High water content-Fresh legume vegetables | IDA31 MRM31 |
| <i>Artemisia selengensis</i> | <i>Artemisia selengensis</i> Turcz. ex Bess. | <i>Asteraceae</i> | Vegetable- Leaf Vegetable- Green leafy vegetables | High water content-Stem and stalk vegetables | IDA3 MRM3 |
| Asparagus | <i>Asparagus officinalis</i> L. | <i>Asparagaceae</i> | Vegetable-Stem | High water content-Stem and stalk vegetables | IDA4 MRM4 |
| Basil | <i>Ocimum basilicum</i> | <i>Lamiaceae</i> | Condiment-Leaf | High water content-Leafy vegetables and fresh herbs | IDA5 MRM5 |

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|-----------------|---|----------------------|---|---|----------------|
| Green tea | / | / | Beverage | High water content-Difficult or unique commodities | IDA16 MRM16 |
| Rosemary | <i>Rosmarinus officinalis</i> | <i>Lamiaceae</i> | Condiment-Leaf | High water content-Stem and stalk vegetables | IDA26 MRM26 |
| Lemon | <i>Citrus limon</i> (L.) Burm. f. | <i>Rutaceae</i> | Fruits- Citrus | High acid content and high water content-Citrus fruit | IDA18 MRM18 |
| Oyster mushroom | <i>Pleurotus ostreatus</i> | <i>Pleurotaceae</i> | Edible fungi- Mushrooms | High water content-Fresh Fungi | IDA23 MRM23 |
| Green chili | <i>Capsicum annuum</i> L. | <i>Solanaceae</i> | Vegetable- Solanaceous Vegetable- Other Solanaceous Vegetable | High water content-fruiting vegetables/cucurbits | IDA14 MRM14 |
| Okra | <i>Abelmoschus esculentus</i> (L.) Moench | <i>Malvaceae</i> | Vegetable- Solanaceous Vegetable- Other Solanaceous Vegetable | High water content-Fruiting vegetables/cucurbits | IDA21 MRM21 |
| Chinese yam | <i>Dioscorea oppositifolia</i> L. | <i>Dioscoreaceae</i> | Vegetable- Tuber vegetable- Other tuber vegetable | High water content-Root and tuber vegetables | IDA9 MRM9 |
| Ginger | <i>Zingiber officinale</i> Roscoe | <i>Zingiberaceae</i> | Vegetable- Rhizomes | High water content-Root and tuber vegetables | IDA13 MRM13 |

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|---------------------------|-------------------------------------|----------------------|----------------------------------|--|----------------|
| Garlic sprout | <i>Allium sativum</i> L. | <i>Liliaceae</i> | Vegetable- Stem brassicas | High water content-Stem and stalk vegetables | IDA12 MRM12 |
| Pea seedlings | <i>Pisum sativum</i> L. | <i>Fabaceae</i> | Vegetable- Sprouts | High water content-Fresh legume vegetables | IDA24 MRM24 |
| Zucchini | <i>Cucurbita pepo</i> L. | <i>Cucurbitaceae</i> | Vegetable- Gourd- Small gourd | High water content-fruiting vegetables/cucurbits | IDA32 MRM32 |
| Maize | <i>Zea mays</i> L. | <i>Poaceae</i> | Cereal- Dry grain | High starch and low water and fat content- Cereal grain and products thereof | IDA19 MRM19 |
| Shiitake mushroom | <i>Lentinus edodes</i> (Berk.) Sing | <i>Omphalotaceae</i> | Edible fungi- Mushrooms | High water content-Fresh Fungi | IDA27 MRM27 |
| Bay leaf | <i>Laurus nobilis</i> L. | <i>Lauraceae</i> | Condiment-Leaf | / | IDA6 MRM6 |
| Cilantro | <i>Coriandrum sativum</i> L. | <i>Apiaceae</i> | Condiment-Leaf | High water content-Leafy vegetables and fresh herbs | IDA10 MRM10 |
| <i>Houttuynia cordata</i> | <i>Herba Houttuyniae</i> | <i>Saururaceae</i> | Medicinal plant- Leaves and stem | High water content-Stem and stalk vegetables | IDA17 MRM17 |

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|-------------------|--|-------------------|---|---|----------------|
| Green Pimiento | <i>Capsicum</i> <i>frutescens</i> L. (syn. <i>C.</i> <i>annuum</i> L.) <i>var.grossum</i> <i>Bailey.</i> | <i>Solanaceae</i> | Vegetable- Solanaceous Vegetable- Other Solanaceous Vegetable | High water content-fruiting vegetables/cucurbits | IDA15 MRM15 |
|-------------------|--|-------------------|---|---|----------------|

Table S3 UHPLC-MS/MS ion transitions, declustering potential (DP), entrance potential (EP), collision energy (CE) and cell exit potential (CXP).

| Precursor ion (m/z) | Product ion (m/z) | ID | DP (V) | EP (V) | CE (eV) | CXP (V) |
|--------------------------------|------------------------------|-----------------|-------------------|-------------------|--------------------|--------------------|
| 270.0 | 238.1 | Alachlor 1 | 41 | 10 | 17 | 14 |
| 270.0 | 162.2 | Alachlor 2 | 41 | 10 | 27 | 10 |
| 270.0 | 146.9 | Alachlor 3 | 41 | 10 | 41 | 18 |
| 228.1 | 68.0 | Ametryn 1 | 156 | 10 | 59 | 8 |
| 228.1 | 96.0 | Ametryn 2 | 156 | 10 | 39 | 26 |
| 228.1 | 91.0 | Ametryn 3 | 156 | 10 | 35 | 10 |
| 215.9 | 174.2 | Atrazine1 | 120 | 10 | 24 | 13 |
| 215.9 | 146.0 | Atrazine 2 | 120 | 10 | 30 | 13 |
| 215.9 | 132.0 | Atrazine 3 | 120 | 10 | 32 | 13 |
| 215.9 | 104.0 | Atrazine 4 | 120 | 10 | 38 | 13 |
| 192.0 | 160.0 | Carbendazim 1 | 41 | 10 | 25 | 10 |
| 192.0 | 132.0 | Carbendazim 2 | 41 | 10 | 41 | 14 |
| 192.0 | 105.0 | Carbendazim 3 | 41 | 10 | 49 | 16 |
| 192.0 | 117.0 | Carbendazim 4 | 41 | 10 | 43 | 14 |
| 192.0 | 133.0 | Carbendazim 5 | 41 | 10 | 41 | 12 |
| 192.0 | 106.1 | Carbendazim 6 | 41 | 10 | 51 | 12 |
| 197.0 | 117.1 | Chlordimeform 1 | 151 | 10 | 37 | 12 |
| 197.0 | 89.0 | Chlordimeform 2 | 151 | 10 | 61 | 12 |
| 197.0 | 90.1 | Chlordimeform 3 | 151 | 10 | 61 | 14 |
| 197.0 | 63.0 | Chlordimeform 4 | 151 | 10 | 81 | 16 |
| 197.0 | 133.0 | Chlordimeform 5 | 151 | 10 | 32 | 16 |
| 197.0 | 106.1 | Chlordimeform 6 | 151 | 10 | 60 | 16 |
| 350.0 | 96.9 | Chlorpyrifos 1 | 82 | 10 | 49 | 9 |
| 350.0 | 197.9 | Chlorpyrifos 2 | 82 | 10 | 29 | 9 |
| 350.0 | 125.0 | Chlorpyrifos 3 | 82 | 10 | 25 | 16 |

| | | | | | | |
|-------|-------|-----------------------|-----|----|----|----|
| 350.0 | 153.0 | Chlorpyrifos 4 | 82 | 10 | 19 | 13 |
| 350.0 | 106.9 | Chlorpyrifos 5 | 82 | 10 | 77 | 12 |
| 321.9 | 145.1 | Chlorpyrifos methyl 1 | 56 | 10 | 19 | 10 |
| 321.9 | 85.1 | Chlorpyrifos methyl 2 | 56 | 10 | 35 | 10 |
| 321.9 | 58.1 | Chlorpyrifos methyl 3 | 56 | 10 | 57 | 8 |
| 359.1 | 167.1 | Chlorsulfuron 1 | 82 | 10 | 29 | 12 |
| 359.1 | 141.1 | Chlorsulfuron 2 | 82 | 10 | 23 | 14 |
| 359.1 | 142.2 | Chlorsulfuron 3 | 82 | 10 | 25 | 8 |
| 359.1 | 168.0 | Chlorsulfuron 4 | 82 | 10 | 25 | 10 |
| 362.9 | 227.0 | Coumaphos 1 | 176 | 10 | 35 | 14 |
| 362.9 | 306.9 | Coumaphos 2 | 176 | 10 | 25 | 18 |
| 362.9 | 335.0 | Coumaphos 3 | 176 | 10 | 21 | 20 |
| 362.9 | 131.1 | Coumaphos 4 | 176 | 10 | 73 | 16 |
| 413.0 | 295.0 | Cyflufenamid 1 | 50 | 10 | 23 | 16 |
| 413.0 | 241.1 | Cyflufenamid 2 | 50 | 10 | 31 | 14 |
| 413.0 | 359.3 | Cyflufenamid 3 | 50 | 10 | 19 | 13 |
| 413.0 | 203.0 | Cyflufenamid 4 | 50 | 10 | 57 | 12 |
| 413.0 | 341.2 | Cyflufenamid 5 | 50 | 10 | 19 | 13 |
| 413.0 | 91.0 | Cyflufenamid 6 | 50 | 10 | 71 | 10 |
| 192.1 | 119.1 | DEET 1 | 91 | 10 | 25 | 6 |
| 192.1 | 91.0 | DEET 2 | 91 | 10 | 41 | 14 |
| 192.1 | 65.1 | DEET 3 | 91 | 10 | 63 | 10 |
| 192.1 | 72.1 | DEET 4 | 91 | 10 | 29 | 8 |
| 305.0 | 169.0 | Diazinon 1 | 120 | 10 | 27 | 11 |
| 305.0 | 153.0 | Diazinon 2 | 120 | 10 | 28 | 11 |
| 220.9 | 109.1 | Dichlorvos 1 | 136 | 10 | 23 | 8 |
| 220.9 | 79.0 | Dichlorvos 2 | 136 | 10 | 39 | 12 |
| 220.9 | 95.0 | Dichlorvos 3 | 136 | 10 | 49 | 12 |
| 220.9 | 60.1 | Dichlorvos 4 | 136 | 10 | 75 | 8 |

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|-------|-------|---------------------|-----|----|-----|----|
| 268.1 | 226.0 | Diethofencarb 1 | 31 | 10 | 15 | 14 |
| 268.1 | 123.9 | Diethofencarb 2 | 31 | 10 | 45 | 14 |
| 268.1 | 180.1 | Diethofencarb 3 | 31 | 10 | 25 | 12 |
| 268.1 | 152.1 | Diethofencarb 4 | 31 | 10 | 31 | 10 |
| 406.1 | 337.0 | Difenoconazole 1 | 120 | 10 | 23 | 7 |
| 406.1 | 251.0 | Difenoconazole 2 | 120 | 10 | 35 | 16 |
| 406.1 | 188.0 | Difenoconazole 3 | 120 | 10 | 61 | 10 |
| 406.1 | 75.0 | Difenoconazole 4 | 120 | 10 | 115 | 10 |
| 406.1 | 111.0 | Difenoconazole 5 | 120 | 10 | 73 | 12 |
| 276.0 | 244.0 | Dimethenamid 1 | 80 | 10 | 21 | 18 |
| 276.0 | 168.1 | Dimethenamid 2 | 80 | 10 | 33 | 10 |
| 276.0 | 111.0 | Dimethenamid 3 | 80 | 10 | 43 | 14 |
| 276.0 | 126.0 | Dimethenamid 4 | 80 | 10 | 47 | 16 |
| 230.0 | 199.0 | Dimethoate 1 | 60 | 10 | 13 | 18 |
| 230.0 | 125.0 | Dimethoate 2 | 60 | 10 | 29 | 14 |
| 230.0 | 171.0 | Dimethoate 3 | 60 | 10 | 21 | 12 |
| 230.0 | 79.0 | Dimethoate 4 | 60 | 10 | 45 | 36 |
| 328.0 | 283.0 | Edifenphos 1 | 90 | 10 | 25 | 16 |
| 328.0 | 109.0 | Edifenphos 2 | 90 | 10 | 49 | 16 |
| 328.0 | 311.3 | Edifenphos 3 | 90 | 10 | 14 | 13 |
| 328.0 | 111.0 | Edifenphos 4 | 90 | 10 | 35 | 14 |
| 328.0 | 173.1 | Edifenphos 5 | 90 | 10 | 32 | 13 |
| 886.2 | 158.1 | Enamectin Benzote 1 | 60 | 10 | 43 | 10 |
| 886.2 | 302.1 | Enamectin Benzote 2 | 60 | 10 | 41 | 20 |
| 886.2 | 126 | Enamectin Benzote 3 | 60 | 10 | 79 | 14 |
| 886.2 | 108.1 | Enamectin Benzote 4 | 60 | 10 | 139 | 12 |
| 886.2 | 98.1 | Enamectin Benzote 5 | 60 | 10 | 117 | 8 |
| 886.2 | 123.0 | Enamectin Benzote 6 | 60 | 10 | 107 | 16 |
| 330.3 | 121.0 | Epoxiconazole 1 | 120 | 10 | 27 | 9 |

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|-------|-------|-----------------|-----|----|-----|----|
| 330.3 | 101.1 | Epoxiconazole 2 | 120 | 10 | 67 | 12 |
| 330.3 | 141.0 | Epoxiconazole 3 | 120 | 10 | 23 | 13 |
| 330.3 | 75.0 | Epoxiconazole 4 | 120 | 10 | 103 | 12 |
| 330.3 | 123.0 | Epoxiconazole 5 | 120 | 10 | 23 | 13 |
| 330.3 | 74.0 | Epoxiconazole 6 | 120 | 10 | 153 | 20 |
| 226.1 | 106.9 | Ethiofencarb 1 | 61 | 10 | 21 | 9 |
| 226.1 | 164.1 | Ethiofencarb 2 | 61 | 10 | 11 | 9 |
| 226.1 | 77.1 | Ethiofencarb 3 | 120 | 10 | 59 | 12 |
| 384.9 | 199.0 | Ethion 1 | 60 | 10 | 15 | 14 |
| 384.9 | 143.1 | Ethion 2 | 60 | 10 | 37 | 12 |
| 384.9 | 97.0 | Ethion 3 | 60 | 10 | 77 | 12 |
| 243.2 | 97.0 | Ethoprophos 1 | 80 | 10 | 47 | 12 |
| 243.2 | 173.2 | Ethoprophos 2 | 80 | 10 | 20 | 13 |
| 243.2 | 130.9 | Ethoprophos 3 | 80 | 10 | 29 | 14 |
| 243.2 | 121.1 | Ethoprophos 4 | 80 | 10 | 31 | 14 |
| 243.2 | 139.0 | Ethoprophos 5 | 80 | 10 | 20 | 13 |
| 243.2 | 201.1 | Ethoprophos 6 | 80 | 10 | 16 | 13 |
| 331.2 | 268.0 | Fenarimol 1 | 161 | 10 | 31 | 16 |
| 331.2 | 111.0 | Fenarimol 2 | 161 | 10 | 79 | 12 |
| 331.2 | 81.0 | Fenarimol 3 | 161 | 10 | 51 | 10 |
| 320.9 | 146.0 | Fenchlorphos 1 | 70 | 10 | 19 | 16 |
| 320.9 | 145.0 | Fenchlorphos 2 | 70 | 10 | 19 | 8 |
| 320.9 | 85.0 | Fenchlorphos 3 | 70 | 10 | 35 | 14 |
| 321.2 | 304.0 | Fenchlorphos 4 | 70 | 10 | 10 | 13 |
| 278.1 | 125.0 | Fenitrothion 1 | 120 | 10 | 28 | 13 |
| 278.1 | 67.1 | Fenitrothion 2 | 120 | 10 | 49 | 18 |
| 278.1 | 108.1 | Fenitrothion 3 | 120 | 10 | 37 | 8 |
| 278.1 | 109.0 | Fenitrothion 4 | 120 | 10 | 43 | 12 |
| 208.1 | 152.0 | Fenobucarb 1 | 65 | 10 | 13 | 9 |

| | | | | | | |
|-------|-------|-------------------|-----|----|-----|----|
| 208.1 | 95.0 | Fenobucarb 2 | 65 | 10 | 19 | 10 |
| 350.3 | 97.2 | Fenpropathrin 1 | 85 | 10 | 46 | 7 |
| 350.3 | 125.1 | Fenpropathrin 2 | 50 | 10 | 25 | 13 |
| 279.0 | 169.1 | Fenthion 1 | 56 | 10 | 25 | 12 |
| 279.1 | 246.8 | Fenthion 2 | 120 | 10 | 18 | 13 |
| 384.0 | 282.1 | Fluazifop butyl 1 | 161 | 10 | 29 | 18 |
| 384.0 | 328.1 | Fluazifop butyl 2 | 161 | 10 | 23 | 22 |
| 384.0 | 254.0 | Fluazifop butyl 3 | 161 | 10 | 39 | 14 |
| 384.0 | 91.0 | Fluazifop butyl 4 | 161 | 10 | 43 | 12 |
| 266.2 | 228.9 | Fludioxonil 1 | 66 | 10 | 23 | 14 |
| 266.2 | 158.0 | Fludioxonil 2 | 66 | 10 | 47 | 16 |
| 266.2 | 185.1 | Fludioxonil 3 | 66 | 10 | 35 | 12 |
| 376.1 | 306.8 | Fluquinconazole 1 | 176 | 10 | 37 | 18 |
| 376.1 | 349.0 | Fluquinconazole 2 | 176 | 10 | 29 | 22 |
| 376.1 | 108.0 | Fluquinconazole 3 | 176 | 10 | 75 | 14 |
| 302.0 | 70.0 | Flutriafol 1 | 71 | 10 | 21 | 10 |
| 302.0 | 123.0 | Flutriafol 2 | 71 | 10 | 39 | 14 |
| 302.0 | 95.0 | Flutriafol 3 | 71 | 10 | 73 | 12 |
| 302.0 | 75.0 | Flutriafol 4 | 71 | 10 | 101 | 10 |
| 353.1 | 228.0 | Hexythiazox 1 | 36 | 10 | 23 | 14 |
| 353.1 | 168.1 | Hexythiazox 2 | 36 | 10 | 35 | 10 |
| 289.0 | 91.0 | Iprobenfos 1 | 51 | 10 | 39 | 14 |
| 289.0 | 205.0 | Iprobenfos 2 | 51 | 10 | 15 | 14 |
| 289.0 | 247.0 | Iprobenfos 3 | 51 | 10 | 11 | 16 |
| 289.0 | 65.1 | Iprobenfos 4 | 51 | 10 | 83 | 10 |
| 314.0 | 162.1 | Isazofos 1 | 186 | 10 | 25 | 10 |
| 314.0 | 97.0 | Isazofos 2 | 186 | 10 | 55 | 12 |
| 314.0 | 120.0 | Isazofos 3 | 70 | 10 | 40 | 9 |
| 314.0 | 119.1 | Isazofos 4 | 186 | 10 | 49 | 6 |

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|-------|-------|--------------------|-----|----|----|----|
| 211.0 | 152.1 | Isoproc carb 1 | 41 | 10 | 17 | 14 |
| 211.0 | 95.0 | Isoproc carb 2 | 25 | 10 | 24 | 7 |
| 331.1 | 127.1 | Malathion 1 | 90 | 10 | 19 | 8 |
| 331.1 | 285.0 | Malathion 2 | 90 | 10 | 11 | 20 |
| 331.1 | 99.0 | Malathion 3 | 90 | 10 | 33 | 12 |
| 331.1 | 125.0 | Malathion 4 | 90 | 10 | 41 | 12 |
| 278.0 | 210.0 | Metazachlor 1 | 50 | 10 | 15 | 13 |
| 278.0 | 134.0 | Metazachlor 2 | 50 | 10 | 30 | 13 |
| 278.0 | 105.1 | Metazachlor 3 | 31 | 10 | 53 | 12 |
| 278.0 | 77.1 | Metazachlor 4 | 31 | 10 | 81 | 14 |
| 280.1 | 220.1 | Metalaxyl 1 | 56 | 10 | 19 | 14 |
| 280.1 | 160.2 | Metalaxyl 2 | 56 | 10 | 33 | 10 |
| 280.2 | 192.3 | Metalaxyl 3 | 56 | 10 | 24 | 11 |
| 141.9 | 94.1 | Methamidophos 1 | 56 | 10 | 23 | 12 |
| 141.9 | 125.0 | Methamidophos 2 | 54 | 10 | 18 | 9 |
| 141.9 | 64.0 | Methamidophos 3 | 56 | 10 | 35 | 10 |
| 303.1 | 145.1 | Methiathion 1 | 121 | 10 | 15 | 10 |
| 303.1 | 85.1 | Methiathion 2 | 121 | 10 | 31 | 38 |
| 264.0 | 232.0 | Methyl Parathion 1 | 46 | 10 | 23 | 16 |
| 264.0 | 75.1 | Methyl Parathion 2 | 46 | 10 | 59 | 12 |
| 284.1 | 252.1 | Metolachlor 1 | 56 | 10 | 21 | 14 |
| 284.1 | 176.2 | Metolachlor 2 | 56 | 10 | 35 | 12 |
| 284.1 | 91.1 | Metolachlor 3 | 56 | 10 | 69 | 10 |
| 284.1 | 77.1 | Metolachlor 4 | 56 | 10 | 97 | 12 |
| 224.0 | 127.0 | Monocrotophos 1 | 126 | 10 | 23 | 16 |
| 224.0 | 98.1 | Monocrotophos 2 | 126 | 10 | 19 | 12 |
| 224.0 | 58.0 | Monocrotophos 3 | 126 | 10 | 41 | 16 |
| 224.0 | 109.1 | Monocrotophos 4 | 126 | 10 | 43 | 14 |
| 289.0 | 70.0 | Myclobutanil 1 | 136 | 10 | 23 | 8 |

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|-------|-------|--------------------------|-----|----|----|----|
| 289.0 | 125.0 | Myclobutanil 2 | 136 | 10 | 49 | 14 |
| 289.0 | 89.0 | Myclobutanil 3 | 136 | 10 | 83 | 10 |
| 214.0 | 125.1 | Omethoate 1 | 111 | 10 | 29 | 4 |
| 214.0 | 155.0 | Omethoate 2 | 111 | 10 | 21 | 10 |
| 214.0 | 109.0 | Omethoate 3 | 111 | 10 | 37 | 16 |
| 214.0 | 182.9 | Omethoate 4 | 56 | 10 | 16 | 6 |
| 279.1 | 219.1 | Oxadixyl 1 | 71 | 10 | 17 | 14 |
| 279.1 | 132.2 | Oxadixyl 2 | 71 | 10 | 45 | 8 |
| 279.1 | 101.9 | Oxadixyl 3 | 100 | 10 | 15 | 13 |
| 279.1 | 117.0 | Oxadixyl 4 | 71 | 10 | 69 | 14 |
| 292.2 | 96.9 | Parathion 1 | 61 | 10 | 53 | 38 |
| 292.2 | 264.0 | Parathion 2 | 60 | 10 | 15 | 13 |
| 282.1 | 212.0 | Pendimethalin 1 | 36 | 10 | 15 | 12 |
| 282.1 | 194.1 | Pendimethalin 2 | 36 | 10 | 25 | 16 |
| 408.0 | 153.1 | Permethrin 1 | 76 | 10 | 65 | 10 |
| 261.0 | 75.0 | Phorate 1 | 51 | 10 | 23 | 10 |
| 261.0 | 96.9 | Phorate 2 | 51 | 10 | 39 | 14 |
| 261.0 | 143.0 | Phorate 3 | 51 | 10 | 25 | 8 |
| 261.0 | 199.0 | Phorate 4 | 51 | 10 | 10 | 10 |
| 293.0 | 247.0 | Phorate sulfone 1 | 120 | 10 | 10 | 13 |
| 293.0 | 171.0 | Phorate sulfone 2 | 120 | 10 | 16 | 13 |
| 276.9 | 171.0 | Phorate-oxon sulfoxide 1 | 80 | 10 | 17 | 13 |
| 276.9 | 199.0 | Phorate-oxon sulfoxide 2 | 56 | 10 | 15 | 12 |
| 276.9 | 153.1 | Phorate-oxon sulfoxide 3 | 80 | 10 | 20 | 13 |
| 276.9 | 97.0 | Phorate-oxon sulfoxide 4 | 56 | 10 | 47 | 12 |
| 276.9 | 143.0 | Phorate-oxon sulfoxide 5 | 56 | 10 | 29 | 14 |
| 276.9 | 78.9 | Phorate-oxon sulfoxide 6 | 56 | 10 | 81 | 10 |
| 367.9 | 182.0 | Phosalone 1 | 56 | 10 | 25 | 12 |
| 367.9 | 111.1 | Phosalone 2 | 56 | 10 | 57 | 10 |

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|-------|-------|----------------------|-----|----|-----|----|
| 367.9 | 75.1 | Phosalone 3 | 56 | 10 | 97 | 12 |
| 367.9 | 74.1 | Phosalone 4 | 56 | 10 | 117 | 8 |
| 367.9 | 322.0 | Phosalone 5 | 120 | 10 | 13 | 13 |
| 318.1 | 256.3 | Phosmet 1 | 60 | 10 | 31 | 16 |
| 318.1 | 160.0 | Phosmet 2 | 60 | 10 | 19 | 30 |
| 318.1 | 77.0 | Phosmet 3 | 60 | 10 | 75 | 8 |
| 300.0 | 174.1 | Phosphamidon 1 | 156 | 10 | 19 | 8 |
| 300.0 | 127.0 | Phosphamidon 2 | 156 | 10 | 31 | 16 |
| 300.0 | 72.1 | Phosphamidon 3 | 156 | 10 | 47 | 8 |
| 300.0 | 108.9 | Phosphamidon 4 | 156 | 10 | 63 | 12 |
| 356.2 | 177.1 | Piperonyl butoxide 1 | 81 | 10 | 19 | 18 |
| 356.2 | 119.1 | Piperonyl butoxide 2 | 81 | 10 | 49 | 14 |
| 356.2 | 147.0 | Piperonyl butoxide 3 | 100 | 10 | 45 | 13 |
| 356.2 | 91.0 | Piperonyl butoxide 4 | 81 | 10 | 75 | 26 |
| 356.2 | 149.0 | Piperonyl butoxide 5 | 81 | 10 | 47 | 18 |
| 306.0 | 164.1 | Pirimiphos methyl 1 | 156 | 10 | 29 | 10 |
| 306.0 | 108.0 | Pirimiphos methyl 2 | 156 | 10 | 41 | 12 |
| 306.0 | 67.0 | Pirimiphos methyl 3 | 156 | 10 | 59 | 8 |
| 306.0 | 125.0 | Pirimiphos methyl 4 | 156 | 10 | 43 | 10 |
| 334.0 | 198.1 | Primiphos ethyl 1 | 6 | 10 | 31 | 12 |
| 334.0 | 182.1 | Primiphos ethyl 2 | 6 | 10 | 31 | 12 |
| 334.0 | 170.1 | Primiphos ethyl 3 | 6 | 10 | 43 | 10 |
| 334.0 | 96.9 | Primiphos ethyl 4 | 6 | 10 | 65 | 12 |
| 372.9 | 302.7 | Profenofos 1 | 156 | 10 | 27 | 22 |
| 372.9 | 344.9 | Profenofos 2 | 156 | 10 | 19 | 22 |
| 372.9 | 128.0 | Profenofos 3 | 156 | 10 | 55 | 16 |
| 372.9 | 97.0 | Profenofos 4 | 156 | 10 | 41 | 16 |
| 242.1 | 158.1 | Prometryne 1 | 221 | 10 | 33 | 10 |
| 242.1 | 200.1 | Prometryne 2 | 221 | 10 | 27 | 12 |

| | | | | | | |
|-------|-------|-------------------|-----|----|----|----|
| 242.1 | 85.0 | Prometryne 3 | 221 | 10 | 43 | 10 |
| 242.1 | 68.1 | Prometryne 4 | 221 | 10 | 99 | 4 |
| 242 | 116.1 | Prometryne 5 | 166 | 10 | 39 | 14 |
| 368.1 | 231.2 | Propargite 1 | 36 | 10 | 15 | 16 |
| 368.1 | 175.2 | Propargite 2 | 36 | 10 | 23 | 4 |
| 230.0 | 188.0 | Propazine 1 | 80 | 10 | 25 | 12 |
| 230.0 | 146.1 | Propazine 2 | 80 | 10 | 33 | 10 |
| 230.0 | 104.0 | Propazine 3 | 80 | 10 | 43 | 12 |
| 230 | 78.9 | Propazine 4 | 80 | 10 | 45 | 12 |
| 344.8 | 240.7 | Prothiofos 1 | 80 | 10 | 25 | 16 |
| 344.8 | 268.9 | Prothiofos 2 | 80 | 10 | 17 | 20 |
| 344.8 | 132.9 | Prothiofos 3 | 80 | 10 | 71 | 16 |
| 344.8 | 160.9 | Prothiofos 4 | 80 | 10 | 47 | 12 |
| 344.8 | 176.9 | Prothiofos 5 | 80 | 10 | 41 | 10 |
| 344.8 | 161.9 | Prothiofos 6 | 80 | 10 | 55 | 12 |
| 365.0 | 308.9 | Pyridaben 1 | 80 | 10 | 19 | 20 |
| 365.0 | 147.1 | Pyridaben 2 | 80 | 10 | 35 | 10 |
| 365.0 | 117.0 | Pyridaben 3 | 80 | 10 | 87 | 14 |
| 365.0 | 98.0 | Pyridaben 4 | 80 | 10 | 61 | 12 |
| 341.0 | 189.1 | Pyridaphenthion 1 | 80 | 10 | 31 | 12 |
| 341.0 | 92.1 | Pyridaphenthion 2 | 80 | 10 | 53 | 10 |
| 341.0 | 65.0 | Pyridaphenthion 3 | 80 | 10 | 75 | 8 |
| 341.0 | 97.0 | Pyridaphenthion 4 | 80 | 10 | 73 | 14 |
| 200.0 | 107.0 | Pyrimethanil 1 | 211 | 10 | 33 | 16 |
| 200.0 | 77.0 | Pyrimethanil 2 | 211 | 10 | 55 | 10 |
| 200.0 | 67.1 | Pyrimethanil 3 | 211 | 10 | 57 | 8 |
| 200.0 | 51.0 | Pyrimethanil 4 | 211 | 10 | 91 | 24 |
| 174.0 | 132.1 | Pyroquilon 1 | 166 | 10 | 33 | 10 |
| 174.0 | 117.1 | Pyroquilon 2 | 166 | 10 | 45 | 12 |

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|-------|-------|-------------------|-----|----|----|----|
| 174.0 | 89.0 | Pyroquilon 3 | 166 | 10 | 75 | 12 |
| 174.0 | 77.0 | Pyroquilon 4 | 166 | 10 | 67 | 10 |
| 299.0 | 97.0 | Quinalphos 1 | 80 | 10 | 49 | 12 |
| 299.0 | 163.1 | Quinalphos 2 | 80 | 10 | 31 | 10 |
| 299.0 | 147.1 | Quinalphos 3 | 80 | 10 | 31 | 10 |
| 299.0 | 119.1 | Quinalphos 4 | 80 | 10 | 59 | 14 |
| 503.0 | 208.1 | Tau Fluvalinate 1 | 80 | 10 | 19 | 14 |
| 503.0 | 181.1 | Tau Fluvalinate 2 | 80 | 10 | 45 | 20 |
| 503.0 | 152.0 | Tau Fluvalinate 3 | 80 | 10 | 99 | 8 |
| 503.0 | 295.1 | Tau Fluvalinate 4 | 80 | 10 | 17 | 13 |
| 258.1 | 125.0 | Thiobencarb 1 | 80 | 10 | 25 | 8 |
| 258.2 | 57.0 | Thiobencarb 2 | 80 | 10 | 47 | 8 |
| 296.1 | 70.0 | Triadimenol 1 | 80 | 10 | 39 | 10 |
| 296.1 | 149.0 | Triadimenol 2 | 80 | 10 | 27 | 10 |
| 314 | 162.1 | Triazophos-1 | 80 | 10 | 25 | 10 |
| 314 | 119.6 | Triazophos-2 | 80 | 10 | 49 | 10 |
| 314 | 120 | Triazophos-3 | 80 | 10 | 35 | 10 |
| 314 | 97 | Triazophos-4 | 80 | 10 | 57 | 10 |
| 318.2 | 70.0 | Triticonazole 1 | 80 | 10 | 55 | 10 |
| 318.2 | 125.1 | Triticonazole 2 | 80 | 10 | 31 | 13 |
| 288.0 | 146.2 | Vamidothion 1 | 80 | 10 | 17 | 10 |
| 288.0 | 118.0 | Vamidothion 2 | 80 | 10 | 35 | 14 |
| 288.0 | 58.0 | Vamidothion 3 | 80 | 10 | 53 | 8 |
| 288.0 | 86.1 | Vamidothion 4 | 80 | 10 | 33 | 10 |

Table S4. Matrix species with pesticides with all their MRM transitions showing MEs > 100% under MRM scan mode.

| Pesticides | Matrix |
|-----------------|--|
| Carbendazim | Basil, Cowpea, Green chili, Maize |
| Difenoconazole | Basil, Cowpea |
| Methiathion | Amaranth, Basil, Blueberry, Cabbage, Chinese yam, Green tea, Green chili, Lemon, Mint, Pea seedling, Red chili, Soybean |
| Myclobutanil | Lemon |
| Propargite | Amaranth, <i>Aritemisia selengensis</i> , Asparagus, Basil, Blueberry, Cabbage, Cowpea, Garlic sprout, Green tea, Mint, Okra, Oyster mushroom, Red chili, Shiitake mushroom, Soybean, Green pimiento |
| Tau-fluvalinate | Soybean |

Table S5. List of 20 pesticides with all their 69 MRM transitions as differential pesticide MRM transitions between groups G1 and G2.

| Chemical classes | Pesticides |
|--------------------------|--|
| Amidoxine | Cyflufenamid |
| Aryloxyphenoxypropionate | Fluazifop-butyl |
| Carboxamide | Hexythiazox |
| Chloroacetamide | Dimethenamid, Alachlor, |
| Organophosphate | Chlorpyrifos, Coumaphos, Diazinon, Dimethoate, Ethion, Isazofos, Parathion, Pirimiphos-methyls, Prothiofos, Quinalphos |
| Sulfonylurea | Chlorsulfuron |
| Triazine | Propazine |
| Triazole | Triadimenol, Triconazole |

Table S6. 13 positive pesticides in corresponding matrices in MS/MS scan under IDA mode by UPLC QTOF

| Pesticide Name | Matrices | MRLs (mg/kg) | Addition level (mg/kg) | S/N | Found at mass (Da) | Error (ppm) | Found at <i>t_R</i> (min) | Library hit | Library score |
|----------------|----------------------------------|-----------------|---------------------------|---------|-----------------------|----------------|--|--------------|------------------|
| Chlorpyrifos | Asparagus | 0.05 | 0.05 | 581.8 | 321.9027 | 1.3 | 11.15 | Chlorpyrifos | 97.7 |
| Chlorpyrifos | Orange | 2 | 0.05 | 682.1 | 321.9028 | 1.6 | 11.07 | Chlorpyrifos | 97.7 |
| Chlorpyrifos | Lemon | 2 | 0.05 | 707.6 | 321.9027 | 1.4 | 11.13 | Chlorpyrifos | 98.2 |
| Chlorpyrifos | Green tea | 2 | 0.625 | 1196 | 321.903 | 2.4 | 11.12 | Chlorpyrifos | 94.7 |
| Chlorpyrifos | Mint | 2 | 0.625 | 686.8 | 321.9031 | 2.7 | 11.13 | Chlorpyrifos | 97.4 |
| Chlorpyrifos | <i>Amomum tsao-ko</i> | 2 | 0.625 | 355.8 | 321.9029 | 1.9 | 11.12 | / | / |
| Chlorpyrifos | Sichuan pepper | 2 | 0.625 | 233.3 | 321.902 | 0.9 | 11.11 | / | / |
| Coumaphos | Orange | 0.05 | 0.05 | 2986.5 | 363.0022 | 1.3 | 10.12 | Coumaphos | 100 |
| Coumaphos | Blueberry | 0.05 | 0.05 | 2028.3 | 363.0222 | 1.4 | 10.11 | Coumaphos | 99.8 |
| Coumaphos | Lemon | 0.05 | 0.05 | 1131.3 | 363.0222 | 1.2 | 10.09 | Coumaphos | 99.7 |
| Coumaphos | Cabbage | 0.05 | 0.05 | 814.5 | 363.0225 | 2.2 | 10.11 | Coumaphos | 99.6 |
| Coumaphos | Wheat grass | 0.05 | 0.05 | 1563 | 363.0223 | 1.5 | 10.13 | Coumaphos | 100 |
| Coumaphos | Red chili | 0.05 | 0.05 | 1701.4 | 363.0227 | 2.7 | 10.15 | Coumaphos | 99.5 |
| Coumaphos | Amaranth | 0.05 | 0.05 | 2390.6 | 363.0223 | 1.5 | 10.17 | Coumaphos | 99.2 |
| Coumaphos | Cowpea | 0.05 | 0.05 | 1178.4 | 363.0226 | 2.3 | 10.11 | Coumaphos | 100 |
| Coumaphos | Winged bean | 0.05 | 0.05 | 40716.4 | 363.0221 | 1.1 | 10.11 | Coumaphos | 99.3 |
| Coumaphos | <i>Artemisia selengensis</i> | 0.05 | 0.05 | 2123.9 | 363.0223 | 1.5 | 10.15 | Coumaphos | 99.6 |
| Coumaphos | Asparagus | 0.05 | 0.05 | 3544.4 | 363.0221 | 1 | 10.18 | Coumaphos | 99.5 |
| Coumaphos | Green chili | 0.05 | 0.05 | 40260.7 | 363.0222 | 1.3 | 10.1 | Coumaphos | 99.7 |
| Coumaphos | Okra | 0.05 | 0.05 | 53195.1 | 363.0226 | 2.5 | 10.11 | Coumaphos | 99.6 |
| Coumaphos | Chinese yam | 0.05 | 0.05 | 41005.6 | 363.0223 | 1.5 | 10.12 | Coumaphos | 99.6 |

| | | | | | | | | | |
|------------|----------------------------------|------|------|---------|----------|-----|-------|------------|------|
| Coumaphos | Ginger | 0.05 | 0.05 | 20611.8 | 363.0231 | 3.8 | 10.11 | Coumaphos | 98.8 |
| Coumaphos | Garlic sprout | 0.05 | 0.05 | 601 | 363.0219 | 0.5 | 10.11 | Coumaphos | 100 |
| Coumaphos | Pea seedling | 0.05 | 0.05 | 996 | 363.0224 | 1.7 | 10.11 | Coumaphos | 100 |
| Coumaphos | Zucchini | 0.05 | 0.05 | 834.4 | 363.0222 | 1.2 | 10.11 | Coumaphos | 100 |
| Coumaphos | Green pimiento | 0.05 | 0.05 | 429979 | 363.0223 | 1.4 | 10.11 | Coumaphos | 100 |
| Dichlorvos | Orange | 0.2 | 0.05 | 773.7 | 220.9534 | 0.9 | 6.88 | Dichlorvos | 96.7 |
| Dichlorvos | Blueberry | 0.2 | 0.05 | 1733.5 | 220.9535 | 1.3 | 6.87 | Dichlorvos | 93.9 |
| Dichlorvos | Lemon | 0.2 | 0.05 | 1770.5 | 220.9533 | 0.6 | 6.89 | Dichlorvos | 98.7 |
| Dichlorvos | Cabbage | 0.5 | 0.05 | 2019.8 | 220.9538 | 2.3 | 6.88 | Dichlorvos | 98.5 |
| Dichlorvos | Wheatgrass | 0.2 | 0.05 | 1596.4 | 220.9533 | 0.6 | 6.85 | Dichlorvos | 99.1 |
| Dichlorvos | Red chili | 0.2 | 0.05 | 1544.7 | 220.953 | 1.5 | 6.85 | Dichlorvos | 97.6 |
| Dichlorvos | Amaranth | 0.2 | 0.05 | 1966.6 | 220.9536 | 1.8 | 6.89 | Dichlorvos | 98.3 |
| Dichlorvos | Cowpea | 0.2 | 0.05 | 1775.7 | 220.9535 | 1.5 | 6.82 | Dichlorvos | 99.2 |
| Dichlorvos | Winged bean | 0.2 | 0.05 | 2006.7 | 220.9534 | 0.9 | 6.83 | Dichlorvos | 96.5 |
| Dichlorvos | <i>Artemisia selengensis</i> | 0.2 | 0.05 | 1706.1 | 220.9536 | 1.8 | 6.84 | / | / |
| Dichlorvos | Asparagus | 0.2 | 0.05 | 2065.1 | 220.9534 | 1 | 6.84 | Dichlorvos | 98.3 |
| Dichlorvos | Green chili | 0.2 | 0.05 | 1895.2 | 220.9533 | 0.5 | 6.84 | Dichlorvos | 99.2 |
| Dichlorvos | Okra | 0.2 | 0.05 | 2079.1 | 220.9535 | 1.6 | 6.85 | Dichlorvos | 99.1 |
| Dichlorvos | Chinese yam | 0.2 | 0.05 | 1940.9 | 220.9532 | 0.1 | 6.89 | Dichlorvos | 100 |
| Dichlorvos | Ginger | 0.2 | 0.05 | 1183.8 | 220.9536 | 1.9 | 6.85 | Dichlorvos | 88.7 |
| Dichlorvos | Garlic sprout | 0.2 | 0.05 | 671.8 | 220.9535 | 1.4 | 6.82 | Dichlorvos | 98.9 |
| Dichlorvos | Pea seedling | 0.2 | 0.05 | 1510.6 | 220.953 | 1.4 | 6.82 | Dichlorvos | 98.5 |
| Dichlorvos | Zucchini | 0.2 | 0.05 | 786.2 | 220.9533 | 0.6 | 6.82 | Dichlorvos | 95.5 |
| Dichlorvos | Green pimiento | 0.2 | 0.05 | 1821.8 | 220.9535 | 1.5 | 6.81 | Dichlorvos | 98.1 |

| | | | | | | | | | |
|---------------|----------------------------------|------|-------|--------|----------|------|-------|---------------|------|
| Epoxiconazole | Orange | 1 | 0.05 | 4069.3 | 330.0802 | -0.5 | 8.82 | Epoxiconazole | 97.7 |
| Fenarimol | Green pimiento | 0.5 | 0.05 | 2166.6 | 331.0407 | 2.4 | 8.65 | Fenarimol | 99.9 |
| Fenthion | Orange | 0.05 | 0.05 | 2713.7 | 279.0279 | 0.9 | 9.85 | Fenthion | 97.7 |
| Fenthion | Blueberry | 0.05 | 0.05 | 3671.8 | 279.0275 | 0.7 | 9.86 | Fenthion | 99.7 |
| Fenthion | Lemon | 0.05 | 0.05 | 1986.1 | 279.0275 | 0.9 | 9.85 | Fenthion | 97.8 |
| Fenthion | Cabbage | 2 | 0.05 | 2213.6 | 279.0277 | 1.4 | 9.85 | Fenthion | 99.1 |
| Fenthion | Wheat grass | 0.05 | 0.05 | 6671.8 | 279.027 | 1.2 | 9.88 | Fenthion | 99.7 |
| Fenthion | Red chili | 0.05 | 0.05 | 3108 | 279.0278 | 1.8 | 9.85 | Fenthion | 99.5 |
| Fenthion | Amaranth | 0.05 | 0.05 | 3069.3 | 279.028 | 2.5 | 9.85 | Fenthion | 97.8 |
| Fenthion | Cowpea | 0.05 | 0.05 | 2250.2 | 279.0278 | 1.9 | 9.85 | Fenthion | 100 |
| Fenthion | Winged bean | 0.05 | 0.05 | 1819.2 | 279.0277 | 1.4 | 9.85 | Fenthion | 99.3 |
| Fenthion | <i>Artemisia selengensis</i> | 0.05 | 0.05 | 1166.9 | 279.0277 | 1.6 | 9.82 | Fenthion | 98.6 |
| Fenthion | Asparagus | 0.05 | 0.05 | 3722.9 | 279.0276 | 1.1 | 9.82 | Fenthion | 96.1 |
| Fenthion | Green chili | 0.05 | 0.05 | 4100.6 | 279.0277 | 1.4 | 9.87 | Fenthion | 98.3 |
| Fenthion | Okra | 0.05 | 0.05 | 7805.3 | 279.0279 | 2.2 | 9.87 | Fenthion | 98.7 |
| Fenthion | Chinese yam | 0.05 | 0.05 | 2622.5 | 279.027 | 1.1 | 9.88 | Fenthion | 97.9 |
| Fenthion | Ginger | 0.05 | 0.05 | 4560 | 279.0279 | 2.2 | 9.82 | Fenthion | 93.4 |
| Fenthion | Garlic sprout | 0.05 | 0.05 | 1270.5 | 279.0276 | 1.2 | 9.82 | Fenthion | 99.2 |
| Fenthion | Pea seedling | 0.05 | 0.05 | 2250.2 | 279.0278 | 1.9 | 9.82 | Fenthion | 100 |
| Fenthion | Zucchini | 0.05 | 0.05 | 2151.9 | 279.0275 | 0.9 | 9.83 | Fenthion | 99.2 |
| Fenthion | Green pimiento | 0.05 | 0.05 | 3340.7 | 279.0276 | 1 | 9.82 | Fenthion | 99.5 |
| Hexythiazox | Orange | 0.5 | 0.05 | 744.7 | 353.1089 | 1.2 | 11.25 | Hexythiazox | 25.8 |
| Hexythiazox | Lemon | 0.5 | 0.05 | 1922.7 | 353.1088 | 0.8 | 11.26 | Hexythiazox | 24.9 |
| Hexythiazox | Green tea | 15 | 0.625 | 2403.4 | 353.109 | 1.5 | 11.25 | Hexythiazox | 12.2 |

| | | | | | | | | | |
|---------------|----------------------------------|------|-------|--------|----------|------|-------|---------------|------|
| Methidathion | Orange | 0.05 | 0.05 | 2806.7 | 302.9709 | 5.8 | 8.53 | / | / |
| Methidathion | Blueberry | 0.05 | 0.05 | 4649.8 | 302.9696 | 1.7 | 8.5 | Methidathion | 99 |
| Methidathion | Lemon | 0.05 | 0.05 | 3563.7 | 302.9689 | -0.7 | 8.5 | / | / |
| Methidathion | Cabbage | 0.05 | 0.05 | 4112.9 | 302.9702 | 3.5 | 8.54 | / | / |
| Methidathion | Wheat grass | 0.05 | 0.05 | 5094.3 | 302.969 | 2.8 | 8.5 | / | / |
| Methidathion | Red chili | 0.05 | 0.05 | 4219.6 | 302.97 | 2.8 | 8.59 | Methidathion | 100 |
| Methidathion | Amaranth | 0.05 | 0.05 | 3392 | 302.9702 | 3.5 | 8.59 | Methidathion | 98.3 |
| Methidathion | Cowpea | 0.05 | 0.05 | 3398.8 | 302.9698 | 2.3 | 8.59 | / | / |
| Methidathion | Winged bean | 0.05 | 0.05 | 4415.7 | 302.9692 | 0.3 | 8.59 | / | / |
| Methidathion | <i>Artemisia selengensis</i> | 0.05 | 0.05 | 1722.6 | 302.9713 | 7.3 | 8.58 | / | / |
| Methidathion | Asparagus | 0.05 | 0.05 | 3820.3 | 302.9698 | 2.2 | 8.54 | / | / |
| Methidathion | Green chili | 0.05 | 0.05 | 4073 | 302.9698 | 2.4 | 8.55 | Methidathion | 100 |
| Methidathion | Okra | 0.05 | 0.05 | 3543.8 | 302.9701 | 3.3 | 8.55 | / | / |
| Methidathion | Chinese yam | 0.05 | 0.05 | 4065.7 | 302.9697 | 1.9 | 8.55 | Methidathion | 100 |
| Methidathion | Ginger | 0.05 | 0.05 | 1378.4 | 302.9705 | 4.6 | 8.53 | / | / |
| Methidathion | Garlic sprout | 0.05 | 0.05 | 82.8 | 302.9697 | 1.9 | 8.53 | / | / |
| Methidathion | Pea seedling | 0.05 | 0.05 | 3253.5 | 32.9699 | 2.5 | 8.52 | / | / |
| Methidathion | Zucchini | 0.05 | 0.05 | 122.1 | 302.9696 | 1.6 | 8.58 | / | / |
| Methidathion | Green pimiento | 0.05 | 0.05 | 3464 | 302.9697 | 1.9 | 8.58 | Methidathion | 96.9 |
| Pendimethalin | Cabbage | 0.5 | 0.05 | 814.5 | 363.0225 | 2.2 | 11.19 | Pendimethalin | 99.6 |
| Pendimethalin | Asparagus | 0.1 | 0.05 | 3544.4 | 363.0221 | 1 | 11.2 | Pendimethalin | 99.5 |
| Phosalone | <i>Amomum tsao-ko</i> | 2 | 0.625 | 204931 | 367.9951 | 2.6 | 10.25 | / | / |
| Phosalone | Sichuan pepper | 2 | 0.625 | 9811.5 | 367.9949 | 2.1 | 10.28 | / | / |
| Phosmet | Orange | 5 | 0.05 | 377.2 | 318.002 | 0.6 | 8.71 | Phosmet | 98.6 |

| | | | | | | | | | |
|-----------------|-------------|------|------|---------|----------|-----|-------|------------|------|
| Phosmet | Lemon | 5 | 0.05 | 443.4 | 318.0026 | 2.4 | 8.75 | Phosmet | 98.4 |
| Phosmet | Blueberry | 10 | 0.05 | 401.3 | 318.0025 | 2 | 8.75 | Phosmet | 97.3 |
| Phosmet | Cabbage | 0.5 | 0.05 | 135.7 | 318.0028 | 3 | 8.7 | Phosmet | 85.7 |
| Profenofos | Cabbage | 0.05 | 0.05 | 56759.2 | 372.9434 | 2.7 | 10.57 | Profenofos | 99.2 |
| Profenofos | Red chili | 3 | 0.05 | 90977.7 | 372.9431 | 1.9 | 10.57 | Profenofos | 99.2 |
| Profenofos | Green chili | 3 | 0.05 | 84789.2 | 372.9429 | 1.3 | 10.57 | Profenofos | 100 |
| Profenofos | Orange | 0.2 | 0.05 | 94685.3 | 372.943 | 1.7 | 10.6 | Profenofos | 99.5 |
| Tau-fluvalinate | Cabbage | 0.5 | 0.05 | 533.6 | 503.1036 | 2.3 | 11.99 | / | / |

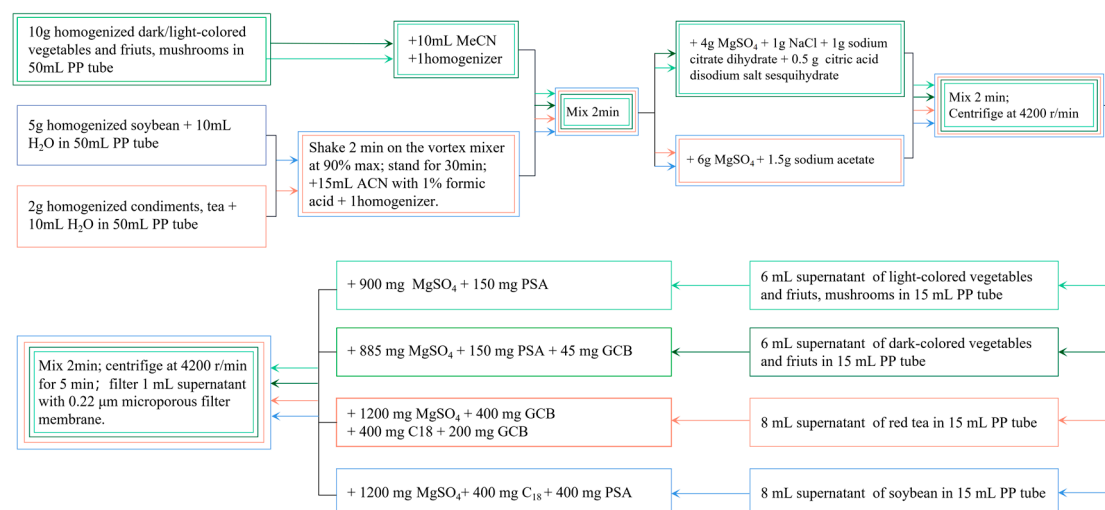


Figure S1. Sample preparation procedures according to the GB 23200.121-2021 National Food

Safety Standard. The flow chart of the QuEChERS cleanup procedure for light fruits and vegetables

and mushrooms were colored in light green, for dark fruits and vegetables was colored in dark green,

for condiments and tea were colored in orange, and for soybeans were colored in blue.

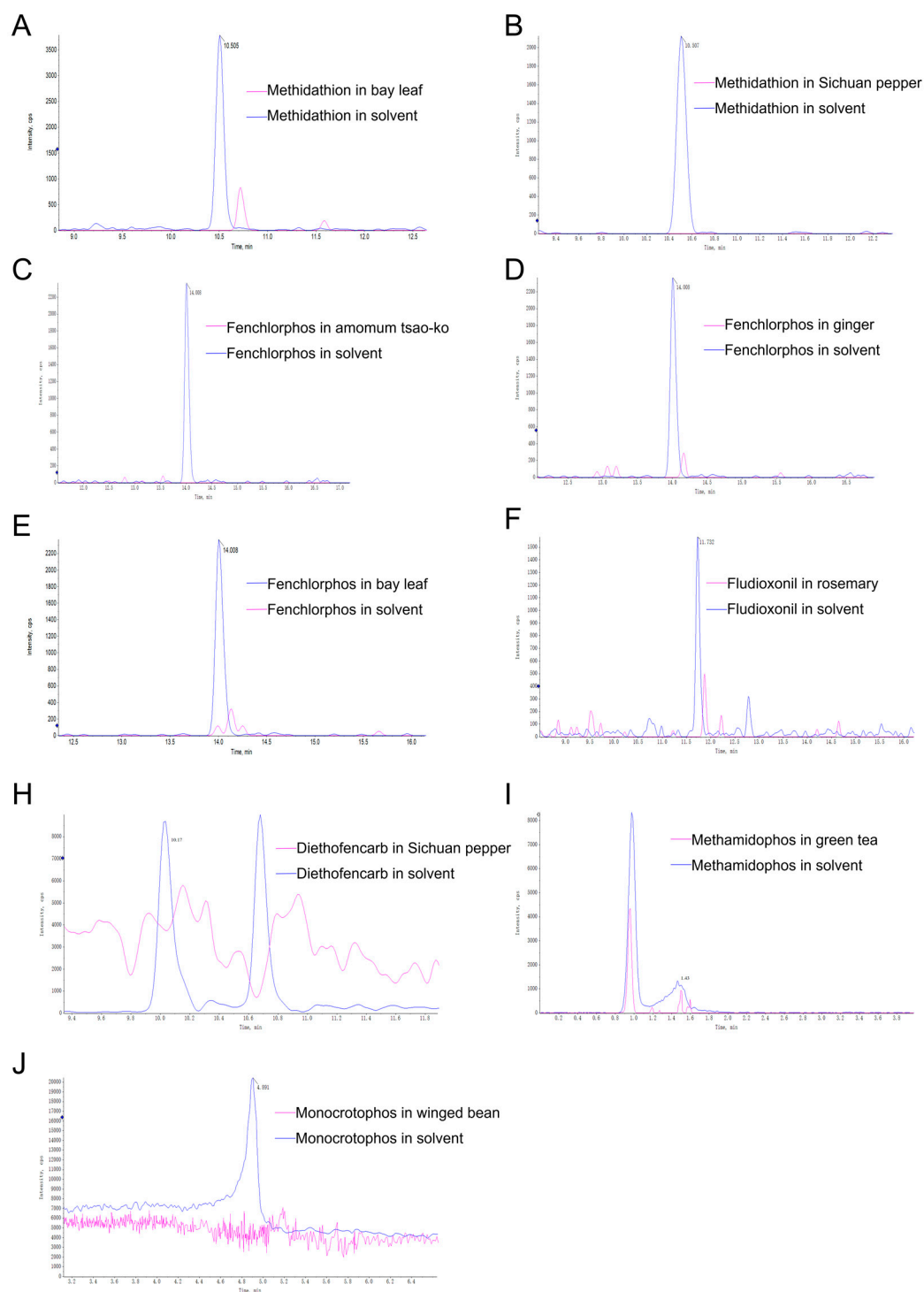


Figure S2. Extracted ion chromatogram (XIC) of pesticides with 100% signal suppression (MEs = -100%) in matrix-matched and reagent-only standard solutions.

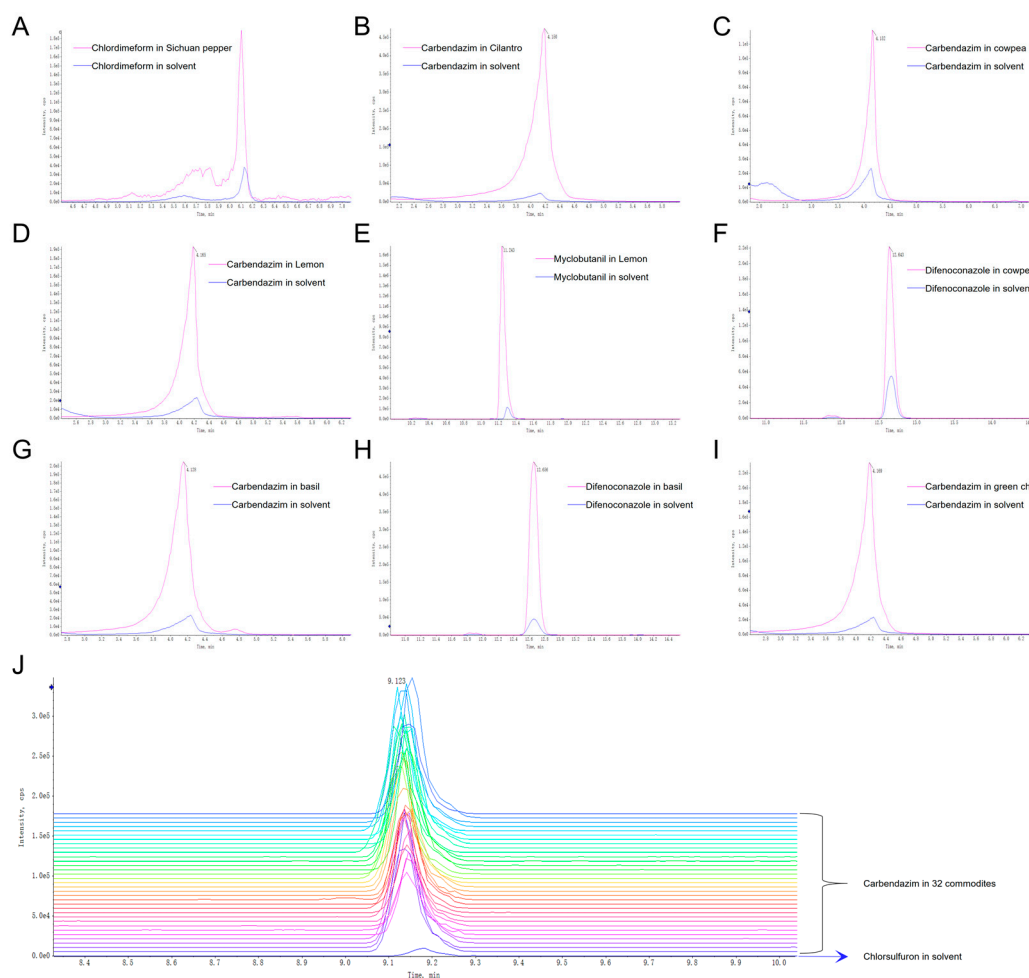


Figure S3. Extracted ion chromatogram (XIC) of pesticides with extreme signal enhancement (MEs > 100%) in matrix-matched and reagent-only standard solutions.

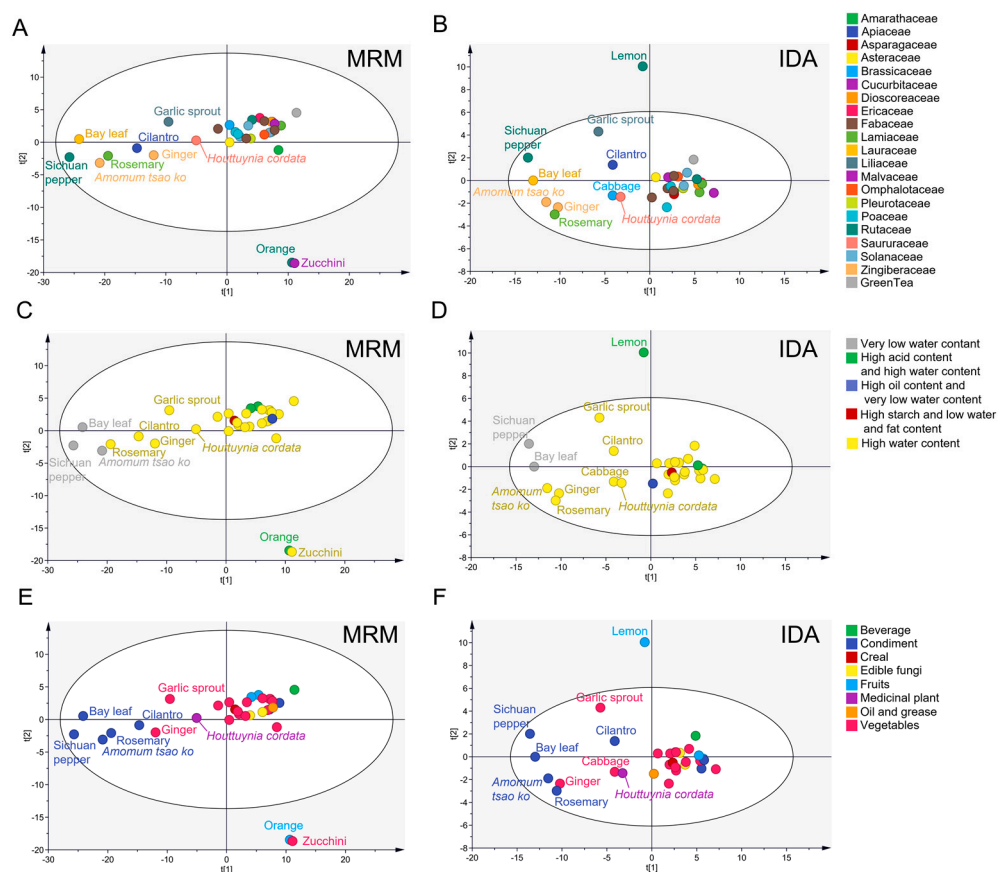


Figure S4. The score plots of PCA modeling under MRM and in TOF-MS scan under IDA mode, colored by botanical classifications (A) and (B), the Document N° SANTE/11312/2021 (C) and (D), and the GB 2763-2021 National Food Safety Standard (E) and (F), respectively.

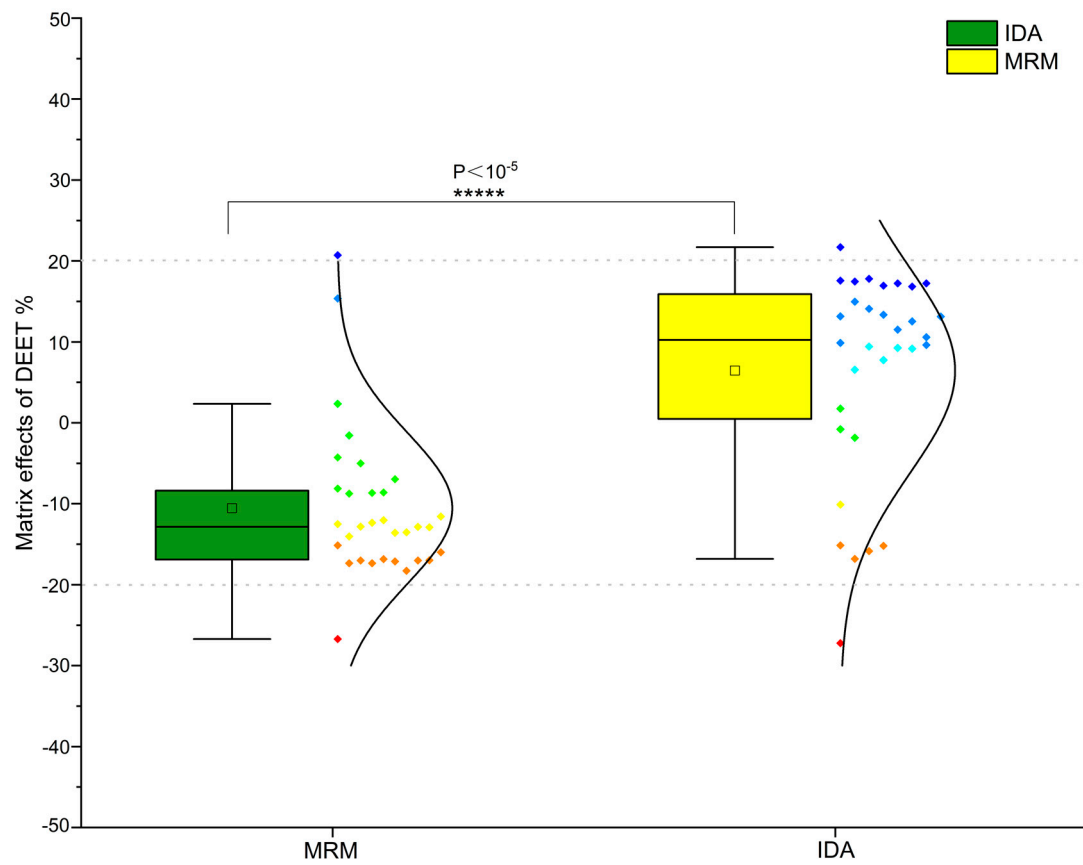


Figure S5. Distribution of DEET's MEs under IDA scan and MRM scan.