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**An enhanced approach for targeted multi-residue screening of pesticides in complex herbal medicines by ultra high-performance liquid chromatography tandem ion mobility/quadrupole time-of-flight mass spectrometry**

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Table S1 Information on eight compounds in a commercial standard solution for the quality control of acquired data

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Component | *m/z* | *t*R/min | Formula | Adducts | CCS/Å2 |
| Caffeine | 195.08765 | 5.00 | C8H10N4O2 | +H | 138.2 |
| Sulfaguanidine | 215.05972 | 2.98 | C7H10N4O2S | +H | 146.8 |
| Sulfadimethoxine | 311.08085 | 5.74 | C12H14N4O4S | +H | 168.4 |
| Val-Tyr-Val | 380.21800 | 5.03 | C19H29N3O5 | +H | 191.7 |
| Verapamil | 455.29043 | 6.68 | C27H38N2O4 | +H | 208.8 |
| Terfenadine | 472.32101 | 10.98 | C32H41NO2 | +H | 228.7 |
| Leucine-Enkephalin | 556.27657 | 5.90 | C28H37N5O7 | +H | 229.8 |
| Reserpine | 609.28066 | 7.67 | C33H40N2O9 | +H | 252.3 |

Table S2 Information on 104 batches of Lonicerae Japonicae Flos samples

|  |  |  |  |
| --- | --- | --- | --- |
| **No.** | **Sample label** | **Collection regions** | **Batch No.** |
| 1 | S1 | Henan Province, China | 20180501 |
| 2 | S2 | Henan Province, China | 20180502 |
| 3 | S4 | Henan Province, China | 20180720 |
| 4 | S5 | Henan Province, China | 20180528 |
| 5 | S6 | Henan Province, China | 20180516 |
| 6 | S8 | Henan Province, China | 20180623 |
| 7 | S9 | Henan Province, China | 20180711 |
| 8 | S10 | Henan Province, China | 20180626 |
| 9 | S14 | Henan Province, China | 160301 |
| 10 | S15 | Henan Province, China | 160302 |
| 11 | S16 | Henan Province, China | 150601 |
| 12 | S17 | Henan Province, China | 150602 |
| 13 | S18 | Henan Province, China | 150901 |
| 14 | S19 | Henan Province, China | 150902 |
| 15 | S20 | Henan Province, China | 170601 |
| 16 | S21 | Henan Province, China | 170602 |
| 17 | S22 | Henan Province, China | 170801 |
| 18 | S23 | Henan Province, China | 170802 |
| 19 | S24 | Henan Province, China | 170803 |
| 20 | S25 | Henan Province, China | 171001 |
| 21 | S26 | Henan Province, China | 171201 |
| 22 | S27 | Henan Province, China | 171202 |
| 23 | S28 | Henan Province, China | 171203 |
| 24 | S29 | Henan Province, China | 180201 |
| 25 | S30 | Henan Province, China | 180202 |
| 26 | S31 | Henan Province, China | 180203 |
| 27 | S32 | Henan Province, China | 180401 |
| 28 | S33 | Henan Province, China | 180402 |
| 29 | S34 | Henan Province, China | 180403 |
| 30 | S35 | Henan Province, China | 180601 |
| 31 | S36 | Henan Province, China | 201805-1 |
| 32 | S37 | Henan Province, China | 201805-2 |
| 33 | S38 | Henan Province, China | 201805-3 |
| 34 | S39 | Henan Province, China | 201805-4 |
| 35 | S40 | Shandong Province, China | 20180503 |
| 36 | S41 | Shandong Province, China | 20180506 |
| 37 | S42 | Shandong Province, China | 20180510 |
| 38 | S43 | Henan Province, China | 201807-1 |
| 39 | S44 | Henan Province, China | 201807-2 |
| 40 | S45 | Henan Province, China | 201807-3 |
| 41 | S46 | Henan Province, China | S160401 |
| 42 | S47 | Hunan Province, China | BZ0101 |
| 43 | S48 | Shandong Province, China | BZ0102 |
| 44 | S49 | Hebei Province, China | BZ0103 |
| 45 | S50 | Hebei Province, China | BZ0104 |
| 46 | S51 | Hebei Province, China | BZ0105 |
| 47 | S52 | Hunan Province, China | BZ0106 |
| 48 | S53 | Shandong Province, China | BZ0107 |
| 49 | S54 | Guizhou Province, China | BZ0108 |
| 50 | S55 | Hunan Province, China | BZ0109 |
| 51 | S56 | Hunan Province, China | BZ0110 |
| 52 | S57 | Hunan Province, China | BZ0111 |
| 53 | S58 | Hunan Province, China | BZ0112 |
| 54 | S59 | Hunan Province, China | BZ0113 |
| 55 | S60 | Hebei Province, China | BZ0114 |
| 56 | S61 | Hunan Province, China | BZ0115 |
| 57 | S62 | Hunan Province, China | BZ0116 |
| 58 | S63 | Hunan Province, China | BZ0117 |
| 59 | S64 | Hubei Province, China | BZ0118 |
| 60 | S65 | Shandong Province, China | YN0101 |
| 61 | S66 | Yunnan Province, China | YN0102 |
| 62 | S67 | Hunan Province, China | YN0103 |
| 63 | S68 | Guizhou Province, China | HX0101 |
| 64 | S69 | Guizhou Province, China | HX0102 |
| 65 | S70 | Chongqing Province, China | HX0103 |
| 66 | S71 | Chongqing Province, China | HX0104 |
| 67 | S72 | Sichuan Province, China | HX0105 |
| 68 | S73 | Sichuan Province, China | HX0106 |
| 69 | S74 | Sichuan Province, China | HX0107 |
| 70 | S75 | Sichuan Province, China | HX0108 |
| 71 | S76 | Sichuan Province, China | HX0109 |
| 72 | S77 | Shandong Province, China | HX0110 |
| 73 | S78 | Shandong Province, China | HX0111 |
| 74 | S79 | Guizhou Province, China | GZ0101 |
| 75 | S80 | Guizhou Province, China | GZ0102 |
| 76 | S81 | Guizhou Province, China | GZ0103 |
| 77 | S82 | Guizhou Province, China | GZ0104 |
| 78 | S83 | Henan Province, China | HB0101 |
| 79 | S84 | Shandong Province, China | HB0102 |
| 80 | S85 | Shandong Province, China | HB0103 |
| 81 | S86 | Hebei Province, China | HB0104 |
| 82 | S87 | Hebei Province, China | HB0105 |
| 83 | S88 | Hebei Province, China | HB0106 |
| 84 | S89 | Hebei Province, China | HZ0101 |
| 85 | S90 | Henan Province, China | HZ0102 |
| 86 | S91 | Sichuan Province, China | HZ0103 |
| 87 | S92 | Henan Province, China | HZ0104 |
| 88 | S93 | Henan Province, China | HZ0105 |
| 89 | S94 | Hebei Province, China | HZ0106 |
| 90 | S97 | Henan Province, China | 190302 |
| 91 | S98 | Shandong Province, China | 20190701 |
| 92 | S99 | Henan Province, China | 191101 |
| 93 | S100 | Henan Province, China | 191102 |
| 94 | S101 | Henan Province, China | 191103 |
| 95 | S01 | Henan Province, China | ZJM-01 |
| 96 | S02 | Henan Province, China | ZJM-02 |
| 97 | S03 | Henan Province, China | ZJM-03 |
| 98 | S04 | Henan Province, China | ZJM-04 |
| 99 | S05 | Henan Province, China | ZJM-05 |
| 100 | S06 | Henan Province, China | ZJM-06 |
| 101 | S07 | Henan Province, China | ZJM-07 |
| 102 | S08 | Henan Province, China | ZJM-08 |
| 103 | S09 | Henan Province, China | ZJM-09 |
| 104 | S010 | Henan Province, China | ZJM-10 |

Table S3 Labile tuning parameter settings

|  |  |
| --- | --- |
| **Parameter** | **Labile Tune** |
| Cone | 30 |
| Source offset | 50 |
| SW1 offset | 5 |
| SW1 pulse heigh | 5 |
| SW2 velocity | 200 |
| MS profile | Cover mass range of analytes e.g., 100/150/200 @25/25/25/25 |
| Ion guide RF gain | 2 |
| Cell2 RF gain | 2 |
| Stepwave RF | 250 |
| Trap/IMS RF | 250 |

Table S4 An Excel template for development of a basic structure library and an example

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Item Name | Synonym "pesticide classification" | Synonym "CAS number" | Item Tag " group" | Structure |
| 1-Naphthyl-acetamide | plant growth regulators | 86-86-2 | 7 | 542.mol\* |

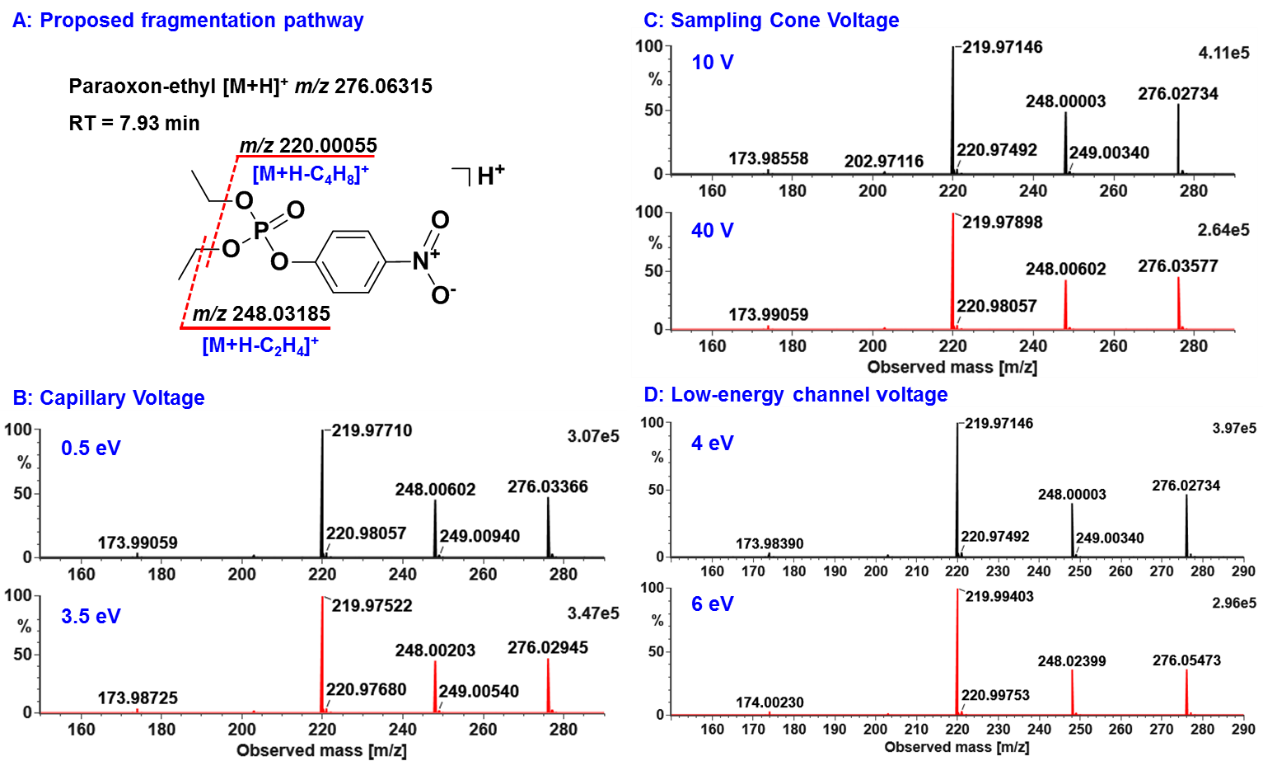
\* 542. mol was the file name of 1-Naphthyl-acetamide in mol..

Table S5 Information on four-dimension identification points of 438 pesticides recorded in the established Pesticide Scientific Library (PSL)

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **No.** | **Item Name** | **Synonym "Chinese Name"** | **Formula** | **Adduct** | **Expected *m/z*** | **CCS** | **t/R** | **F1** | **F2** | **F3** | **F4** | **F5** |
| 1 | Abamectin-B1a | 阿维菌素 | C48H72O14 | +Na | 895.48143 | 299.09 | 17.05 | 449.25338 | 305.21112 | 521.28977 | 549.32107 | 567.33163 |
| 2 | Acetamiprid | 啶虫脒 | C10H11ClN4 | +H | 223.07450 | 150.37 | 5.57 | 126.01050 | 90.03383 |  |  |  |
| 3 | Acetochlor | 乙草胺 | C14H20ClNO2 | +H | 270.12553 | 155.78 | 11.53 | 224.08367 | 59.04914 | 148.11208 |  |  |
| 4 | Akton | 硫虫畏 | C12H14Cl3O3PS | +H | 374.95396 | 167.80 | 14.85 | 169.96846 | 204.93731 | 96.95076 | 346.92266 | 318.89136 |
| 5 | Aldicarb-sulfone | 涕灭威砜 | C7H14N2O4S | +Na | 245.05665 | 147.22 | 4.55 | 86.06004 | 81.00048 | 76.03930 |  |  |
| 6 | Alloxydim | 禾草灭 | C17H25NO5 | +H | 324.18055 | 175.81 | 11.83 | 192.10191 | 164.10699 | 234.11247 | **266.13868** | 178.04987 |
| 7 | Ametoctradin | 苯唑嘧菌胺 | C15H25N5 | +H | 276.21827 | 175.59 | 13.49 | 176.09307 | 149.08217 | 190.10872 |  |  |
| 8 | Ametryn | 莠灭净 | C9H17N5S | +H | 228.12774 | 154.13 | 9.58 | 186.08079 | 158.04949 | 144.05899 | 116.02769 | 68.02432 |
| 9 | Amicarbazone | 胺唑草酮 | C10H19N5O2 | +Na | 264.14310 | 168.75 | 6.74 | 165.07468 |  |  |  |  |
| 10 | Aminocarb | 灭害威 | C11H16N2O2 | +H | 209.12845 | 150.17 | 4.49 | 122.06004 | 137.08352 | 152.10699 |  |  |
| 11 | Anilofos | 莎稗磷 | C13H19ClNO3PS2 | +H | 368.03053 | 177.78 | 12.28 | 124.98206 | 170.96978 | 166.00542 | 198.96470 |  |
| 12 | Atrazine | 阿特拉津 | C8H14ClN5 | +H | 216.10105 | 149.13 | 8.35 | 174.05410 | 146.02280 | 132.03230 | 104.00100 | 138.07742 |
| 13 | Atrazine-desethyl | 脱乙基阿特拉津 | C6H10ClN5 | +H | 188.06975 | 139.86 | 5.98 | 146.02280 | 110.04612 | 104.00100 | 68.02432 |  |
| 14 | Atrazine-desisopropyl | 脱异丙基莠去津 | C5H8ClN5 | +H | 174.05410 | 132.82 | 5.35 | 68.02432 | 146.02280 | 104.00100 |  |  |
| 15 | Azaconazole | 氧环唑 | C12H11Cl2N3O2 | +H | 300.03011 | 161.55 | 8.80 | 158.97628 | 230.99741 |  |  |  |
| 16 | Azamethiphos | 甲基吡啶磷 | C9H10ClN2O5PS | +H | 324.98093 | 158.34 | 6.60 | 182.99558 | 139.00575 | 111.99485 |  |  |
| 17 | Azimsulfuron | 四唑嘧磺隆 | C13H16N10O5S | +H | 425.10986 | 192.22 | 8.14 | 182.05602 | 139.05020 | 227.03457 | 156.07675 | 244.06112 |
| 18 | Azinphos-ethyl | 乙基谷硫磷(益棉磷) | C12H16N3O3PS2 | +Na | 368.02629 | 174.80 | 11.29 | 77.03858 | 132.04439 | 232.94905 | 289.01165 | 137.00556 |
| 19 | Azinphos-methyl | 甲基谷硫磷(保棉磷) | C10H12N3O3PS2 | +Na | 339.99499 | 167.00 | 9.22 | 132.04439 | 77.03858 | 124.98206 | 105.03349 |  |
| 20 | Aziprotryne | 叠氮津 | C7H11N7S | +H | 226.08694 | 146.93 | 10.86 | 184.06514 | 198.08079 | 156.03384 | 142.04334 | 111.05395 |
| 21 | Azoxystrobin | 腈嘧菌酯 | C21H14N3O4 | -e | 372.09788 | 186.54 | 9.65 | 329.07949 | 344.10297 | 328.07167 | 172.03930 |  |
| 22 | Beflubutamid | 氟丁酰草胺 | C18H17F4NO2 | +H | 356.12682 | 180.92 | 11.99 | 91.05423 | 193.02710 |  |  |  |
| 23 | Benalaxyl | 苯霜灵 | C20H23NO3 | +H | 326.17507 | 171.74 | 12.40 | 148.11208 | 133.08860 | 208.13321 | 294.14886 | 266.15394 |
| 24 | Benfuracarb | 丙硫克百威 | C20H30N2O5S | +H | 411.19482 | 198.95 | 13.94 | 195.04340 | 162.06753 | 252.06889 | 158.11756 |  |
| 25 | Benodanil | 麦锈灵 | C13H10INO | +H | 323.98798 | 148.62 | 8.03 | 202.93522 | 230.93013 | 76.03075 |  |  |
| 26 | Benoxacor | 解草嗪 | C11H11Cl2NO2 | +H | 260.02396 | 146.85 | 9.49 | 134.06004 | 160.07569 | 120.04439 | 149.08352 |  |
| 27 | Bensulfuron-methyl | 苄嘧磺隆 | C16H18N4O7S | +H | 411.09690 | 187.86 | 9.26 | 182.05602 | 149.05971 | 119.04914 | 91.05423 | 139.05020 |
| 28 | Bensulide | 地散磷 | C14H24NO4PS3 | +Na | 420.04973 | 189.38 | 11.83 | 141.00048 | 77.03858 | 200.01983 | 158.02703 | 218.03040 |
| 29 | Benthiavalicarb-isopropyl | 苯噻菌胺 | C18H24FN3O3S | +H | 382.15952 | 188.54 | 10.72 | 180.02777 | 197.05432 | 116.07060 |  |  |
| 30 | Benzoximate | 苯螨特 | C18H18ClNO5 | +Na | 386.07657 | 189.10 | 12.88 | 199.01565 | 183.99217 | 170.00033 | 140.97378 |  |
| 31 | Benzoylprop-ethyl | 新燕灵 | C18H17Cl2NO3 | +Na | 388.04777 | 192.94 | 12.55 | 77.03858 | 105.03349 | 292.02905 | 320.02396 |  |
| 32 | Benzyladenine | 苄腺嘌呤 | C12H11N5 | +H | 226.10872 | 148.38 | 6.39 | 148.06177 | 91.05423 |  |  |  |
| 33 | Bispyribac | 双草醚 | C19H18N4O8 | +H | 431.11974 | 198.07 | 10.29 | 275.06625 | 413.10918 | 243.04003 | 381.08296 | 139.05020 |
| 34 | Boscalid | 啶酰菌胺 | C18H12Cl2N2O | +H | 343.03994 | 172.65 | 10.49 | 271.08659 | 307.06327 | 111.99485 | 139.98977 |  |
| 35 | Bromfenvinfos | 溴苯烯磷 | C12H14BrCl2O4P | +H | 402.92629 | 167.30 | 12.71 | 169.96846 | 98.98417 | 80.97361 | 248.88679 | 155.04677 |
| 36 | Brompyrazon | 溴莠敏 | C10H8BrN3O | +H | 265.99235 | 141.86 | 5.81 | 186.06619 | 189.96105 | 236.97838 | 172.93450 | 92.04948 |
| 37 | Bromuconazole,cis | 糠菌唑 | C13H12BrCl2N3O | +H | 375.96136 | 168.45 | 11.06 | 158.97628 | 172.95555 | 144.96063 | 70.03997 |  |
| 38 | Bromuconazole,trans | 糠菌唑 | C13H12BrCl2N3O | +H | 375.96136 | 169.61 | 12.13 | 158.97628 | 172.95555 | 144.96063 | 70.03997 |  |
| 39 | Bupirimate | 乙嘧酚磺酸酯 | C13H24N4O3S | +H | 317.16419 | 174.52 | 11.65 | 210.16009 | 166.09749 | 208.14444 | 272.10634 | 150.10257 |
| 40 | Buprofezin | 噻嗪酮 | C16H23N3OS | +H | 306.16346 | 173.05 | 14.43 | 106.06513 | 77.03858 | 201.10561 |  |  |
| 41 | Butafenacil | 氟丙嘧草酯 | C20H18ClF3N2O6 | +NH4 | 492.11437 | 211.55 | 11.10 | 331.00918 | 179.98468 | 123.99485 | 151.98977 | 349.01975 |
| 42 | Butralin | 仲丁灵 | C14H21N3O4 | +H | 296.16048 | 168.90 | 15.70 | 222.08732 | 178.07368 | 208.07167 | 240.09788 |  |
| 43 | Buturon | 炔草隆 | C12H13ClN2O | +H | 237.07892 | 152.30 | 8.52 | 207.03197 | 126.01050 | 93.05730 | 222.05544 |  |
| 44 | Cafenstrole | 唑草胺 | C16H22N4O3S | +Na | 373.13048 | 191.03 | 10.95 | 119.08553 | 105.06988 | 72.04439 | 100.07569 | 252.08012 |
| 45 | Carbetamide | 双酰草胺 | C12H16N2O3 | +H | 259.10531 | 164.83 | 6.49 | 92.04948 | 120.04439 | 77.03858 | 192.06552 |  |
| 46 | Carbosulfan | 丁硫克百威 | C20H32N2O3S | +H | 381.22064 | 189.86 | 17.20 | 128.14338 | 160.11545 | 123.04406 | 76.02155 | 118.06850 |
| 47 | Carboxin | 萎锈灵 | C12H13NO2S | +H | 236.07398 | 149.72 | 7.31 | 93.05730 | 143.01613 |  |  |  |
| 48 | Carfentrazone-ethyl | 唑草酮 | C15H14Cl2F3N3O3 | +H | 412.04371 | 180.00 | 12.08 | 345.99561 | 276.97415 | 302.03025 | 366.00184 |  |
| 49 | Carpropamid | 加普胺 | C15H18Cl3NO | +H | 334.05267 | 172.82 | 12.35 | 103.05423 | 77.03858 | 139.03090 | 102.04640 | 160.05237 |
| 50 | Chlorantraniliprole | 氯虫酰胺 | C18H14BrCl2N5O2 | +Na | 503.96001 | 204.52 | 9.11 | 283.92208 | 450.93587 | 177.00883 | 194.00033 | 205.00374 |
| 51 | Chlorbromuron | 氯溴隆 | C9H10BrClN2O2 | +H | 292.96869 | 151.53 | 10.56 | 204.92884 | 182.02414 | 125.00268 | 203.92102 | 153.02140 |
| 52 | Chlorfenvinphos | 毒虫畏 | C12H14Cl3O4P | +H | 358.97681 | 164.95 | 12.48 | 169.96846 | 98.98417 | 80.97361 | 204.93731 | 155.04677 |
| 53 | Chloridazon | 氯草敏 | C10H8ClN3O | +H | 222.04287 | 141.31 | 5.71 | 193.02889 | 146.01157 | 77.03858 | 104.04948 | 92.04948 |
| 54 | Chlorimuron-ethyl | 氯嘧磺隆 | C15H15ClN4O6S | +H | 415.04736 | 192.63 | 10.58 | 186.00648 | 121.02841 | 184.99031 | 143.00067 |  |
| 55 | Chloroxuron | 枯草隆 | C15H15ClN2O2 | +H | 291.08948 | 172.10 | 11.14 | 218.03672 | 72.04439 | 183.06787 |  |  |
| 56 | Chlorphoxim | 氯辛硫磷 | C12H14ClN2O3PS | +H | 333.02240 | 166.89 | 12.63 | 138.01050 | 102.03383 | 110.99960 | 249.94890 | 163.00575 |
| 57 | Chlorpyrifos | 毒死蜱 | C9H11Cl3NO3PS | +H | 349.93356 | 163.90 | 15.07 | 197.92747 | 161.95080 | 96.95076 | 275.86040 | 293.87096 |
| 58 | Chlorpyrifos-methyl | 甲基毒死蜱 | C7H7Cl3NO3PS | +H | 321.90226 | 152.84 | 13.36 | 289.87605 | 124.98206 |  |  |  |
| 59 | Chlorpyrifos-oxon | 氧毒死蜱 | C9H11Cl3NO4P | +H | 333.95640 | 159.69 | 11.75 | 197.92747 | 277.89380 | 161.95080 | 259.88324 | 133.95588 |
| 60 | Chlorsulfuron | 氯磺隆 | C12H12ClN5O4S | +H | 358.03713 | 175.76 | 6.94 | 167.05635 | 141.07709 | 83.02399 | 110.99960 |  |
| 61 | Chlortoluron | 绿麦隆 | C10H13ClN2O | +H | 213.07892 | 145.79 | 8.05 | 72.04439 | 140.02615 |  |  |  |
| 62 | Cinidon-ethyl | 吲哚酮草酯 | C19H17Cl2NO4 | +H | 394.06074 | 192.99 | 14.47 | 348.01888 | 239.96136 | 213.98210 | 366.02944 |  |
| 63 | Cinosulfuron | 醚磺隆 | C15H19N5O7S | +H | 414.10780 | 191.62 | 6.22 | 183.05127 | 280.02608 | 83.02399 | 157.07200 |  |
| 64 | Clethodim | 烯草酮 | C17H26ClNO3S | +H | 360.13947 | 189.76 | 13.78 | 166.08626 | 164.07061 | 136.07569 | 149.05971 | 268.13658 |
| 65 | Clodinafop-propargyl | 炔草酯 | C17H13ClFNO4 | +H | 350.05899 | 179.47 | 12.02 | 222.01165 | 238.04295 | 238.06656 | 266.03786 | 91.05423 |
| 66 | Clomazone | 异恶草酮 | C12H14ClNO2 | +H | 240.07858 | 145.89 | 9.45 | 125.01525 | 89.03858 |  |  |  |
| 67 | Cloransulam-methyl | 氯酯磺草胺 | C15H13ClFN5O5S | +H | 430.03827 | 189.60 | 7.02 | 306.01886 | 369.98076 | 152.99759 | 398.01206 | 185.02381 |
| 68 | Coumaphos | 蝇毒磷 | C14H16ClO5PS | +H | 363.02174 | 180.36 | 12.46 | 226.99263 | 288.94857 | 211.01565 | 225.98480 | 306.95913 |
| 69 | Coumaphos-oxon | 氧蝇毒磷 | C14H16ClO6P | +H | 347.04458 | 175.40 | 9.29 | 211.01565 | 272.97141 | 290.98198 | 319.01328 | 209.00000 |
| 70 | Coumatetralyl | 杀鼠醚 | C19H16O3 | +H | 293.11722 | 162.84 | 11.10 | 121.02841 | 91.05423 | 175.03897 |  |  |
| 71 | Crimidine | 鼠立死 | C7H10ClN3 | +H | 172.06360 | 131.73 | 6.19 | 136.08692 | 109.07602 | 80.04948 | 120.05562 | 95.06037 |
| 72 | Crufomate | 育畜磷 | C12H19ClNO3P | +H | 292.08638 | 163.47 | 11.84 | 236.02378 | 203.99757 | 260.06017 | 108.02089 | 230.99723 |
| 73 | Cumyluron | 苄苯隆 | C17H19ClN2O | +H | 303.12587 | 165.26 | 10.95 | 185.04762 | 125.01525 | 91.05423 | 119.08553 |  |
| 74 | Cyanazine | 氰草净 | C9H13ClN6 | +H | 241.09630 | 154.71 | 6.46 | 214.08540 | 174.05410 | 132.03230 | 104.00100 |  |
| 75 | Cyazofamid | 氰霜唑 | C13H13ClN4O2S | +H | 325.05205 | 164.92 | 11.54 | 216.03230 | 182.07127 | 155.06037 | 164.02615 | 108.01138 |
| 76 | Cycluron | 环锈隆 | C11H22N2O | +H | 199.18049 | 148.39 | 8.90 | 72.04439 | 89.07094 | 69.06988 |  |  |
| 77 | Cyflufenamid | 环氟菌胺 | C20H17F5N2O2 | +H | 413.12830 | 182.01 | 12.67 | 203.02269 | 221.03325 | 183.01646 | 241.03948 | 295.08643 |
| 78 | Cyhalothrin | 氯氟氰菊酯 | C23H19ClF3NO3 | +Na | 472.08978 | 207.66 | 15.64 | 181.06479 | 141.05103 | 225.02885 | 161.05726 |  |
| 79 | Cymiazole | 螨蜱胺 | C12H14N2S | +H | 219.09505 | 147.10 | 5.64 | 171.09167 | 203.06375 | 156.06820 | 130.06513 | 144.08078 |
| 80 | Cyprazine | 环丙津 | C9H14ClN5 | +H | 228.10105 | 151.80 | 8.48 | 144.03230 | 186.05410 | 108.05562 | 150.07742 |  |
| 81 | Cyproconazole-1 | 环唑醇(环丙唑醇) | C15H18ClN3O | +H | 292.12112 | 168.00 | 11.23 | 125.01525 | 70.03997 |  |  |  |
|  | Cyproconazole-2 | 环唑醇(环丙唑醇) | C15H18ClN3O | +H | 292.12112 | 167.14 | 10.87 | 125.01525 | 70.03997 |  |  |  |
| 82 | Cyprodinil | 嘧菌环胺 | C14H15N3 | +H | 226.13387 | 152.62 | 12.21 | 210.10257 | 77.03858 | 93.05730 | 108.08078 |  |
| 83 | Cyprofuram | 酯菌胺 | C14H14ClNO3 | +H | 280.07350 | 159.98 | 7.41 | 130.06513 | 166.04180 | 184.05237 |  |  |
| 84 | Cyprosulfamide | 环丙磺酰胺 | C18H18N2O5S | +H | 375.10092 | 191.47 | 6.32 | 135.04406 | 254.08117 | 121.02841 | 77.03858 |  |
| 85 | Cythioate | 畜蜱磷 | C8H12NO5PS2 | +H | 297.99673 | 160.42 | 6.05 | 154.97150 | 233.94430 | 265.97051 | 184.98206 | 217.00828 |
| 86 | DEET | 避蚊胺 | C12H17NO | +H | 192.13829 | 143.17 | 8.36 | 91.05423 | 119.04914 |  |  |  |
| 87 | Demeton-S-methyl-sulfoxide | 磺吸磷 | C6H15O4PS2 | +H | 247.02221 | 141.45 | 4.72 | 109.00491 | 124.98206 | 169.00828 | 105.03686 |  |
| 88 | Demeton-S-methyl-sulphon | 砜吸磷 | C6H15O5PS2 | +H | 263.01713 | 142.97 | 4.86 | 124.98206 | 169.00828 | 78.99434 | 109.00491 |  |
| 89 | Desmedipham | 甜菜胺 | C16H16N2O4 | +Na | 323.10023 | 179.02 | 8.80 | 136.03930 | 108.04439 | 93.03349 | 154.04987 | 182.08117 |
| 90 | Diallate | 燕麦敌 | C10H17Cl2NOS | +H | 270.04807 | 155.29 | 13.72 | 108.96063 | 106.97168 | 72.98395 |  |  |
| 91 | Diazinon | 二嗪磷 | C12H21N2O3PS | +H | 305.10833 | 170.62 | 12.49 | 169.07940 | 153.10224 | 96.95076 | 84.04439 |  |
| 92 | Diazinon-O-analog | 二嗪磷氧同系物 | C12H21N2O4P | +H | 289.13117 | 168.56 | 9.14 | 153.10224 | 233.06857 | 84.04439 | 261.09987 |  |
| 93 | Dichlorfenthion | 除线磷 | C10H13Cl2O3PS | +H | 314.97728 | 157.06 | 14.83 | 222.93801 | 258.91468 | 204.92744 | 240.90412 | 162.97120 |
| 94 | Dichlorvos | 敌敌畏 | C4H7Cl2O4P | +H | 220.95318 | 133.93 | 6.79 | 109.00491 | 127.01547 | 78.99452 |  |  |
| 95 | Diclobutrazol | 苄氯三唑醇 | C15H19Cl2N3O | +H | 328.09779 | 171.96 | 12.14 | 158.97628 | 70.03997 |  |  |  |
| 96 | Diclosulam | 双氯磺草胺 | C13H10Cl2FN5O3S | +H | 405.99382 | 181.80 | 7.34 | 160.97936 | 125.00268 | 377.96252 |  |  |
| 97 | Dicrotophos | 百治磷 | C8H16NO5P | +H | 238.08389 | 147.81 | 5.09 | 109.00491 | 127.01547 | 193.02604 |  |  |
| 98 | Diethatyl-ethyl | 乙酰甲草胺 | C16H22ClNO3 | +H | 312.13610 | 168.01 | 11.97 | 147.10425 | 132.08078 | 162.12773 | 117.05730 | 238.09932 |
| 99 | Diethofencarb | 乙霉威 | C14H21NO4 | +Na | 290.13628 | 177.36 | 9.93 | 124.03930 | 152.07061 | 108.04439 | 180.10191 | 226.10738 |
| 100 | Difenoconazole | 苯醚甲环唑 | C19H17Cl2N3O3 | +H | 406.07197 | 199.36 | 13.22 | 251.00250 | 188.03873 | 223.00758 | 337.03928 |  |
| 101 | Difenoxuron | 枯秀隆 | C16H18N2O3 | +H | 287.13902 | 174.21 | 8.52 | 214.08626 | 95.04914 | 186.09134 | 72.04439 | 123.04406 |
| 102 | Difenzoquat-methyl-sulfate | 野燕枯 | C17H17N2 | -e | 249.13862 | 159.74 | 5.56 | 193.08860 | 233.10732 | 130.06513 | 234.11515 |  |
| 103 | Diflufenican | 吡氟酰草胺 | C19H11F5N2O2 | +H | 395.08135 | 186.95 | 13.45 | 266.04234 | 246.03611 | 238.04742 | 218.04120 | 233.05210 |
| 104 | Dimefuron | 恶唑隆 | C15H19ClN4O3 | +H | 339.12184 | 191.14 | 9.30 | 167.00067 | 139.98977 | 212.05852 | 72.04439 |  |
| 105 | Dimethachlor | 二甲草胺 | C13H18ClNO2 | +H | 256.10988 | 150.25 | 9.05 | 148.11208 | 224.08367 | 132.08078 | 105.06988 | 118.06513 |
| 106 | Dimethametryn | 异戊乙净 | C11H21N5S | +H | 256.15904 | 164.97 | 11.92 | 186.08079 | 158.04949 | 138.07742 | 144.05899 | 116.02769 |
| 107 | Dimethenamid | 二甲吩草胺 | C12H18ClNO2S | +H | 276.08195 | 154.16 | 10.36 | 168.08415 | 244.05574 | 111.02630 | 152.05285 | 126.03720 |
| 108 | Dimethomorph-1 | 烯酰吗啉 | C21H22ClNO4 | +H | 388.13101 | 199.81 | 10.14 | 301.06260 | 165.05462 | 273.06768 | 258.04421 |  |
|  | Dimethomorph-2 | 烯酰吗啉 | C21H22ClNO4 | +H | 388.13101 | 200.47 | 10.71 | 301.06260 | 165.05462 | 273.06768 | 258.04421 |  |
| 109 | Dimethylvinphos | 甲基毒虫畏 | C10H10Cl3O4P | +H | 330.94550 | 157.61 | 11.05 | 169.96846 | 127.01547 | 109.00491 | 204.93731 |  |
| 110 | Dimetilan | 敌蝇威 | C10H16N4O3 | +H | 241.12952 | 153.30 | 5.64 | 72.04439 | 151.01382 | 196.07167 |  |  |
| 111 | Dimoxystrobin | 醚菌胺 | C19H22N2O3 | +H | 327.17032 | 172.54 | 12.06 | 223.09917 | 238.12264 | 116.04948 | 280.13321 | 89.03858 |
| 112 | Diniconazole | 烯唑醇 | C15H17Cl2N3O | +H | 326.08214 | 174.16 | 13.25 | 70.03997 | 158.97628 | 252.00898 | 204.07003 |  |
| 113 | Dinitramine | 氨氟灵 | C11H13F3N4O4 | +H | 323.09617 | 158.76 | 12.90 | 215.06648 | 247.04374 | 289.09069 | 261.05939 | 305.08560 |
| 114 | Dioxathion-1 | 敌杀磷 | C8H16O4PS2 | -e | 271.02221 | 145.80 | 14.13 | 96.95076 | 128.92283 | 140.97698 | 78.94020 | 184.98543 |
|  | Dioxathion-2 | 敌杀磷 | C8H16O4PS2 | -e | 271.02221 | 146.15 | 14.34 | 96.95076 | 128.92283 | 140.97698 | 184.98543 |  |
| 115 | Diphenamid | 双苯酰草胺 | C16H17NO | +H | 240.13829 | 153.56 | 8.95 | 134.09643 | 167.08553 |  |  |  |
| 116 | Dipropetryn | 异丙净 | C11H21N5S | +H | 256.15904 | 165.78 | 12.01 | 144.03384 | 214.11209 | 186.08079 | 172.06514 | 102.01204 |
| 117 | Disulfoton sulfone | 乙拌磷砜 | C8H19O4PS3 | +H | 307.02558 | 156.16 | 7.95 | 96.95076 | 78.94020 | 171.02393 | 260.98372 |  |
| 118 | Dithiopyr | 氟硫草定 | C15H16F5NO2S2 | +H | 402.06154 | 176.87 | 13.55 | 271.99876 | 248.03292 | 296.03629 | 223.99762 | 354.05817 |
| 119 | Diuron | 敌草隆 | C9H10Cl2N2O | +H | 233.02429 | 147.00 | 8.86 | 159.97153 | 125.00268 | 72.04439 |  |  |
| 120 | Dodemorph | 十二环吗淋 | C18H35NO | +H | 282.27914 | 176.16 | 8.84 | 116.10699 | 98.09643 |  |  |  |
| 121 | Dodine | 多果定 | C13H29N3 | +H | 228.24342 | 176.59 | 12.82 | 186.22163 | 211.21688 |  |  |  |
| 122 | Doramectin | 多拉菌素 | C50H74O14 | +Na | 921.49708 | 306.68 | 17.78 | 777.42084 | 331.22677 | 593.34728 | 575.33672 | 833.44705 |
| 123 | Drazoxolon | 肼菌酮 | C10H8ClN3O2 | +H | 238.03778 | 146.04 | 11.38 | 130.06513 | 177.02140 | 220.02722 | 142.05255 |  |
| 124 | Edifenphos | 克瘟散 | C14H15O2PS2 | +H | 311.03238 | 159.54 | 12.25 | 109.01065 | 154.97150 | 77.03858 | 172.98206 | 283.00108 |
| 125 | Emamectin B1A Benzoate | 甲氨基阿维菌素 | C49H75NO13 | +H | 886.53112 | 300.03 | 14.68 | 158.11756 | 82.06513 | 868.52055 | 302.19620 |  |
| 126 | EPN | 苯硫膦 | C14H14NO4PS | +H | 324.04539 | 167.59 | 13.40 | 156.98715 | 262.02637 | 278.00353 | 138.97658 | 261.03347 |
| 127 | Eprinomectin B1a | 依立诺克丁 | C50H75NO14 | +Na | 936.50798 | 309.09 | 16.61 | 154.08626 | 144.10191 | 199.11174 | 298.16490 |  |
| 128 | Esprocarb | 戊草丹 | C15H23NOS | +H | 266.15731 | 159.92 | 14.40 | 91.05423 | 196.07906 |  |  |  |
| 129 | Etaconazole | 乙环唑 | C14H15Cl2N3O2 | +H | 328.06141 | 172.15 | 11.43 | 158.97628 |  |  |  |  |
| 130 | Ethametsulfuron-methyl | 胺苯磺隆 | C15H18N6O6S | +H | 411.10813 | 197.64 | 7.30 | 168.05160 | 83.02399 | 196.08290 | 142.07234 | 135.04406 |
| 131 | Ethidimuron | 磺噻隆 | C7H12N4O3S2 | +H | 265.04236 | 151.45 | 5.35 | 208.02089 | 116.02769 | 74.00590 | 116.02769 | 161.97903 |
| 132 | Ethiprole | 乙虫腈 | C13H9Cl2F3N4OS | +H | 396.98990 | 182.66 | 10.36 | 254.96981 | 350.94803 | 227.95892 |  |  |
| 133 | Ethirimol | 乙嘧酚 | C11H19N3O | +H | 210.16009 | 151.76 | 7.06 | 182.12879 | 140.10699 | 193.13354 | 165.10224 | 98.06004 |
| 134 | Ethoprophos | 灭线磷 | C8H19O2PS2 | +H | 243.06368 | 148.55 | 11.44 | 215.03238 | 96.95076 | 78.94020 | 172.98543 | 130.93848 |
| 135 | Ethoxysulfuron | 乙氧磺隆 | C15H18N4O7S | +H | 399.09690 | 187.56 | 10.77 | 139.03763 | 261.02882 | 154.06110 | 182.05602 |  |
| 136 | Etobenzanid | 乙氧苯草胺 | C16H15Cl2NO3 | +H | 340.05018 | 178.80 | 12.44 | 121.02841 | 93.03349 | 149.05971 | 282.00831 | 179.07027 |
| 137 | Etoxazole | 乙螨唑 | C21H23F2NO2 | +H | 360.17696 | 186.50 | 15.40 | 141.01465 | 113.01973 | 304.11436 | 177.12739 |  |
| 138 | Famphur | 伐灭磷 | C10H16NO5PS2 | +H | 326.02803 | 168.79 | 7.74 | 154.97150 | 217.00828 | 171.97424 | 184.98206 | 201.98480 |
| 139 | Fenamidone | 咪唑菌酮 | C17H17N3OS | +H | 312.11651 | 170.35 | 10.23 | 236.11822 | 134.07262 | 150.02462 | 92.04948 | 264.11314 |
| 140 | Fenamiphos | 苯线磷 | C13H22NO3PS | +H | 304.11308 | 169.64 | 11.79 | 201.98480 | 217.00828 | 234.03483 | 184.98206 | 276.08178 |
| 141 | Fenamiphos sulfone | 苯线磷砜 | C13H22NO5PS | +H | 336.10291 | 179.08 | 6.87 | 188.04711 | 266.02466 | 170.03654 | 308.07161 |  |
| 142 | Fenamiphos sulfoxide | 苯线磷亚砜 | C13H22NO4PS | +H | 320.10799 | 179.87 | 6.69 | 233.00319 | 216.00045 | 154.04469 | 217.97972 |  |
| 143 | Fenarimol | 氯苯嘧啶醇 | C17H12Cl2N2O | +H | 331.03994 | 173.85 | 11.34 | 268.05237 | 189.06988 | 138.99452 | 278.06053 |  |
| 144 | Fenazaquin | 喹螨醚 | C20H22N2O | +H | 307.18049 | 172.74 | 16.53 | 147.05529 | 131.08553 | 161.13248 | 146.10900 | 91.05423 |
| 145 | Fenbuconazole | 腈苯唑 | C19H17ClN4 | +H | 337.12145 | 183.43 | 11.66 | 125.01525 | 70.03997 | 128.06205 |  |  |
| 146 | Fenchlorphos oxon | 氧皮蝇磷 | C8H8Cl3O4P | +H | 304.92985 | 153.15 | 11.40 | 257.88017 | 272.90364 | 109.00491 | 127.01547 |  |
| 147 | Fenfuram | 甲呋酰胺 | C12H11NO2 | +H | 202.08626 | 141.55 | 7.53 | 109.02841 |  |  |  |  |
| 148 | Fenhexamid | 环酰菌胺 | C14H17Cl2NO2 | +H | 302.07091 | 164.19 | 11.32 | 143.01324 | 142.00542 | 177.98210 | 97.10118 |  |
| 149 | Fenoxaprop-ethyl | 精恶唑禾草灵 | C18H16ClNO5 | +H | 362.07898 | 189.40 | 14.04 | 288.04220 | 91.05423 |  |  |  |
| 150 | Fenoxycarb | 苯氧威 | C17H19NO4 | +H | 302.13868 | 178.85 | 11.89 | 256.09682 | 116.07060 | 88.03930 |  |  |
| 151 | Fenpiclonil | 拌种咯 | C11H6Cl2N2 | +H | 236.99808 | 149.54 | 9.36 | 202.02923 | 140.04948 | 166.05255 | 174.01050 | 201.02140 |
| 152 | Fenpropidin | 苯锈啶 | C19H31N | +H | 274.25293 | 166.85 | 9.07 | 147.11683 | 117.06988 | 119.08553 | 132.09335 |  |
| 153 | Fenpyrazamine | 胺苯吡菌酮 | C17H21N3O2S | +H | 332.14272 | 177.86 | 10.94 | 216.11314 | 230.12879 | 189.08966 | 130.06513 | 272.17574 |
| 154 | Fenpyroximate | 唑螨酯 | C24H27N3O4 | +H | 422.20743 | 215.45 | 15.80 | 366.14483 | 214.09749 | 199.08659 | 107.04914 | 138.06619 |
| 155 | Fensulfothion | 丰索磷 | C11H17O4PS2 | +H | 309.03786 | 171.97 | 8.28 | 234.96470 | 218.98754 | 140.02904 | 157.03178 | 252.97526 |
| 156 | Fensulfothion-oxon | 氧丰索磷 | C11H17O5PS | +H | 293.06071 | 168.03 | 5.88 | 236.99811 | 218.98754 | 140.02904 | 201.98480 | 174.00765 |
| 157 | Fensulfothion-oxon-sulfone | 氧丰索磷砜 | C11H17O6PS | +H | 309.05562 | 168.72 | 5.97 | 175.01547 | 252.99302 | 157.00491 | 281.02432 |  |
| 158 | Fensulfothion-sulfone | 丰索磷砜 | C11H17O5PS2 | +H | 325.03278 | 170.54 | 8.58 | 190.99263 | 268.97018 | 172.98206 | 94.04132 | 173.02669 |
| 159 | Fenthion | 倍硫磷 | C10H15O3PS2 | +H | 279.02730 | 155.01 | 12.36 | 168.98715 | 121.01065 | 105.06988 | 247.00108 | 153.03686 |
| 160 | Fenthion-oxon-sulfoxide | 氧倍硫磷亚砜 | C10H15O5PS | +H | 279.04506 | 161.81 | 5.44 | 264.02158 | 247.01884 | 216.05460 |  |  |
| 161 | Fenthion-sulfone | 倍硫磷砜 | C10H15O5PS2 | +H | 311.01713 | 165.72 | 7.23 | 168.98715 | 246.96470 | 278.99901 | 167.97932 | 200.00554 |
| 162 | Fenthion-sulfoxide | 倍硫磷亚砜 | C10H15O4PS2 | +H | 295.02221 | 164.73 | 6.95 | 279.99874 | 168.98715 | 262.99600 | 232.03175 |  |
| 163 | Ferimzone | 嘧菌腙 | C15H18N4 | +H | 255.16042 | 164.40 | 10.03 | 117.05730 | 124.08692 | 91.05423 | 132.08078 | 163.09782 |
| 164 | Fipronil-sulfone | 氟虫腈砜MB46136 | C12H4Cl2F6N4O2S | +Na | 474.92284 | 197.36 | 12.27 | 243.97764 | 319.98379 | 242.96981 | 212.94802 |  |
| 165 | Flamprop-isopropyl | 麦草氟异丙酯 | C19H19ClFNO3 | +H | 364.11103 | 180.94 | 12.32 | 77.03858 | 105.03349 | 172.03238 | 136.05570 | 276.05860 |
| 166 | Flazasulfuron | 嘧啶磺隆 | C13H12F3N5O5S | +H | 408.05840 | 182.19 | 9.04 | 182.05602 | 139.05020 | 146.02121 | 227.00966 | 156.07675 |
| 167 | Flonicamid | 氟啶虫酰胺 | C9H6F3N3O | +H | 230.05357 | 146.46 | 4.94 | 148.03686 | 146.02121 | 176.03177 | 203.04267 | 183.03645 |
| 168 | Florasulam | 双氟磺草胺 | C12H8F3N5O3S | +H | 360.03727 | 170.21 | 5.90 | 129.03846 | 109.03223 | 128.03063 | 108.02440 | 130.04112 |
| 169 | Fluazifop-p-butyl | 精吡氟禾草灵 | C19H20F3NO4 | +H | 384.14172 | 196.67 | 14.06 | 282.07364 | 238.04742 | 328.07912 | 91.05423 | 254.07873 |
| 170 | Fluazuron | 吡虫隆 | C20H10Cl2F5N3O3 | +H | 506.00921 | 205.76 | 15.00 | 348.97529 | 141.01465 | 158.04120 |  |  |
| 171 | Flubendiamide | 氟虫双酰胺 | C23H22F7IN2O4S | +Na | 705.01254 | 224.07 | 11.88 | 273.93595 | 147.03148 | 407.97610 | 103.04165 | 570.97479 |
| 172 | Flucarbazone | 氟酮磺隆 | C12H11F3N4O6S | +H | 397.04242 | 174.52 | 5.64 | 130.06110 | 115.03763 |  |  |  |
| 173 | Flucycloxuron | 氟环脲 | C25H20ClF2N3O3 | +Na | 506.10535 | 219.07 | 15.28 | 132.04439 | 141.01465 | 289.07831 | 104.04948 |  |
| 174 | Flucythrinate | 氟氰戊菊酯 | C26H23F2NO4 | +NH4 | 469.19334 | 212.30 | 15.11 | 181.06479 | 157.04595 | 412.15433 | 107.04914 |  |
| 175 | Flufenacet | 氟噻草胺 | C14H13F4N3O2S | +Na | 386.05568 | 186.93 | 11.31 | 124.05570 | 152.05062 | 97.04480 | 109.04480 | 194.09757 |
| 176 | Flufenpyr-ethyl | 氟哒嗪草酯 | C16H13ClF4N2O4 | +H | 409.05727 | 181.83 | 11.75 | 335.02049 | 307.02558 | 271.04890 |  |  |
| 177 | Flumetsulam | 唑嘧磺草胺 | C12H9F2N5O2S | +H | 326.05178 | 164.97 | 5.34 | 129.03846 | 109.03223 | 144.02555 | 262.08988 |  |
| 178 | Flumiclorac-pentyl | 胺氟草酯 | C21H23ClFNO5 | +NH4 | 424.13216 | 208.15 | 14.22 | 308.04843 | 280.05351 | 288.04220 | 174.01165 | 354.05390 |
| 179 | Flumioxazin | 丙炔氟草胺 | C19H15FN2O4 | +H | 355.10886 | 185.71 | 9.15 | 299.08265 | 327.11395 | 259.05135 | 313.09830 | 176.05062 |
| 180 | Fluometuron | 氟草隆 | C10H11F3N2O | +H | 233.08962 | 147.04 | 7.74 | 145.02596 | 168.02555 | 160.03686 | 140.03063 |  |
| 181 | Fluopicolide | 氟吡菌胺 | C14H8Cl3F3N2O | +H | 382.97271 | 172.87 | 10.69 | 172.95555 | 144.96063 | 193.99789 | 108.98395 | 364.96214 |
| 182 | Fluopyram | 氟吡菌酰胺 | C16H11ClF6N2O | +H | 397.05369 | 175.11 | 11.09 | 208.01354 | 145.02596 | 173.02088 | 172.03686 |  |
| 183 | Fluoroglycofen-ethyl | 乙羧氟草醚 | C18H13ClF3NO7 | +Na | 470.02248 | 208.18 | 13.50 | 222.97682 | 300.00337 | 343.99320 | 178.98699 | 279.99714 |
| 184 | Fluoxastrobin | 氟嘧菌酯 | C21H16ClFN4O5 | +H | 459.08660 | 204.15 | 11.13 | 427.06039 | 188.03804 | 306.06733 | 367.03926 | 383.03417 |
| 185 | Fluquinconazole | 氯喹唑 | C16H8Cl2FN5O | +H | 376.01627 | 180.30 | 11.23 | 306.98357 | 272.01472 | 349.00537 | 163.03022 |  |
| 186 | Fluridone | 氟啶草酮 | C19H14F3NO | +H | 330.11003 | 178.15 | 9.32 | 309.09597 | 290.09757 | 259.09917 | 275.07409 |  |
| 187 | Flurochloridone | 氟咯草酮 | C12H10Cl2F3NO | +H | 312.01643 | 160.14 | 10.99 | 292.01020 | 212.06816 | 198.05251 | 240.06307 | 174.05251 |
| 188 | Flurprimidol | 抑嘧醇 | C15H15F3N2O2 | +H | 313.11584 | 170.06 | 10.74 | 269.05324 | 185.07094 | 242.04234 | 189.01579 |  |
| 189 | Flurtamone | 呋草酮 | C18H14F3NO2 | +H | 334.10494 | 177.13 | 10.02 | 247.07291 | 178.07770 | 227.06668 | 275.06783 |  |
| 190 | Flusilazole | 氟硅唑 | C16H15F2N3Si | +H | 316.10761 | 173.13 | 11.77 | 165.06968 | 219.04361 | 247.07491 | 227.06868 | 151.03738 |
| 191 | Fluthiacet-methyl | 嗪草酸甲酯 | C15H15ClFN3O3S2 | +H | 404.03002 | 186.79 | 12.15 | 239.02850 | 214.98405 | 344.00889 | 273.99736 | 331.00106 |
| 192 | Flutolanil | 氟酰胺 | C17H16F3NO2 | +H | 324.12059 | 172.50 | 10.63 | 242.06118 | 262.06741 | 145.02596 | 282.07364 |  |
| 193 | Flutriafol | 粉唑醇 | C16H13F2N3O | +H | 302.10994 | 163.77 | 8.09 | 95.02915 | 109.04480 | 123.02407 | 70.03997 |  |
| 194 | Fluxapyroxad | 氟唑菌酰胺 | C18H12F5N3O | +H | 382.09733 | 174.65 | 10.71 | 342.08487 | 314.08996 | 234.05251 | 271.06034 | 206.03379 |
| 195 | Foramsulfuron | 甲酰胺磺隆 | C17H20N6O7S | +H | 453.11869 | 199.69 | 7.17 | 182.05602 | 255.04340 | 139.05020 | 212.00120 | 227.01210 |
| 196 | Forchlorfenuron | 福芬素 | C12H10ClN3O | +H | 248.05852 | 153.07 | 8.74 | 129.02140 | 93.04472 | 155.00067 | 119.02399 |  |
| 197 | Fosthiazate | 噻唑膦 | C9H18NO3PS2 | +H | 284.05385 | 154.23 | 7.64 | 104.01646 | 96.95076 | 199.95995 | 227.99125 |  |
| 198 | Fuberidazole | 麦穗宁 | C11H8N2O | +H | 185.07094 | 134.77 | 5.94 | 157.07602 | 156.06820 | 119.06037 | 118.05255 | 92.04948 |
| 199 | Furalaxyl | 呋霜灵 | C17H19NO4 | +H | 302.13868 | 162.04 | 9.78 | 242.11756 | 95.01276 | 270.11247 |  |  |
| 200 | Furametpyr | 福拉比 | C17H20ClN3O2 | +H | 334.13168 | 176.80 | 7.99 | 157.01632 | 290.10547 | 254.12879 | 186.09134 | 131.03705 |
| 201 | Furathiocarb | 呋线威 | C18H26N2O5S | +H | 383.16352 | 191.98 | 14.20 | 162.06753 | 195.04743 | 252.06889 | 167.05251 |  |
| 202 | Furmecyclox | 拌种胺 | C14H21NO3 | +H | 252.15942 | 157.05 | 12.38 | 123.04406 | 170.08117 | 110.06004 |  |  |
| 203 | Griseofulvin | 灰黄霉素 | C17H17ClO6 | +H | 353.07864 | 179.64 | 7.85 | 215.01056 | 165.05462 | 285.05243 |  |  |
| 204 | Halofenozide | 氯虫酰肼 | C18H19ClN2O2 | +Na | 353.10273 | 186.95 | 10.28 | 105.03349 | 138.99452 | 275.05818 |  |  |
| 205 | Haloxyfop-2-ethoxyethyl | 氟吡乙禾磷 | C19H19ClF3NO5 | +H | 434.09766 | 187.31 | 14.06 | 316.03467 | 288.00337 | 272.00845 | 260.04728 | 344.02958 |
| 206 | Haloxyfop-methyl | 氟吡甲禾磷 | C16H13ClF3NO4 | +H | 376.0558 | 184.13 | 13.33 | 272.00845 | 316.03467 | 288.00337 |  |  |
| 207 | Heptenophos | 庚烯磷 | C9H12ClO4P | +H | 251.02345 | 143.65 | 8.65 | 127.01547 | 125.01525 | 109.00491 | 89.03858 | 215.04677 |
| 208 | Hexazinone | 环嗪酮 | C12H20N4O2 | +H | 253.16590 | 159.38 | 7.02 | 171.08765 | 85.07602 | 71.06037 | 114.06619 | 101.03455 |
| 209 | Hexythiazox | 噻螨酮 | C17H21ClN2O2S | +Na | 375.09045 | 184.29 | 15.08 | 168.05745 | 115.05020 | 116.05803 | 151.03090 | 228.02444 |
| 210 | Hydramethylnon | 氟蚁腙 | C25H24F6N4 | +H | 495.19779 | 240.70 | 13.05 | 323.14781 | 368.08685 | 238.05866 | 151.03538 |  |
| 211 | Imazalil | 烯菌灵 | C14H14Cl2N2O | +H | 297.05559 | 165.27 | 8.07 | 158.97628 | 255.00864 | 172.99193 | 200.98685 |  |
| 212 | Imazamethabenz-methyl | 咪草酸 | C16H20N2O3 | +H | 289.15467 | 168.00 | 6.93 | 144.04439 | 161.07094 | 116.04948 | 215.08150 | 229.13354 |
| 213 | Imazamox | 甲氧咪草烟 | C15H19N3O4 | +H | 306.14483 | 171.42 | 5.61 | 246.08732 | 193.06077 | 163.05020 | 218.09240 | 261.12337 |
| 214 | Imazapic | 甲咪唑烟酸 | C14H17N3O3 | +H | 276.13427 | 161.69 | 5.74 | 163.05020 | 216.07675 | 145.03964 | 188.08184 |  |
| 215 | Imazaquin | 灭草喹 | C17H17N3O3 | +H | 312.13427 | 170.95 | 6.62 | 199.05020 | 181.03964 | 198.06619 | 153.04472 | 252.07675 |
| 216 | Imazethapyr | 咪草烟 | C15H19N3O3 | +H | 290.14992 | 167.63 | 6.26 | 177.06585 | 230.09240 | 159.05529 | 202.09749 | 245.12845 |
| 217 | Imazosulfuron | 唑吡嘧磺隆(依速隆) | C14H13ClN6O5S | +H | 413.04294 | 187.49 | 10.45 | 257.97347 | 231.99420 | 153.02140 | 156.07675 | 182.05602 |
| 218 | Imibenconazole | 亚胺唑 | C17H13Cl3N4S | +H | 410.99993 | 189.01 | 14.62 | 125.01525 | 181.98257 | 89.03858 | 251.01527 |  |
| 219 | Imidacloprid-guanidine | 吡虫啉 | C9H11ClN4 | +H | 211.07450 | 146.62 | 4.21 | 126.01050 | 90.03383 | 175.09782 | 133.07602 | 91.04165 |
| 220 | Imidacloprid-urea | 吡虫啉脲 | C9H10ClN3O | +H | 212.05852 | 141.67 | 5.28 | 128.02615 | 126.01050 | 127.01833 | 93.05730 | 90.03383 |
| 221 | Indanofan | 茚草酮 | C20H17ClO3 | +Na | 363.07584 | 180.64 | 11.47 | 175.07536 | 323.08333 | 173.05971 | 131.04914 |  |
| 222 | Indaziflam | 茚嗪氟草胺 | C16H20FN5 | +H | 302.17755 | 177.52 | 11.58 | 138.07742 | 145.10118 | 158.08365 |  |  |
| 223 | Iodosulfuron-methyl | 甲基碘磺隆 | C14H14IN5O6S | +H | 507.97822 | 198.17 | 8.69 | 167.05635 | 260.94070 | 324.90260 | 389.89142 | 141.07709 |
| 224 | Iprovalicarb | 异丙菌胺 | C18H28N2O3 | +Na | 343.19921 | 182.93 | 11.07 | 119.08553 | 116.07061 | 203.13902 |  |  |
| 225 | Isocarbophos | 水胺硫磷 | C11H16NO4PS | +Na | 312.04299 | 165.73 | 8.50 | 121.02841 | 137.00556 | 230.98754 | 154.97150 | 93.03349 |
| 226 | Isofenphos | 异硫磷 | C7H6O4PS | -e | 216.97189 | 137.88 | 12.87 | 121.02841 |  |  |  |  |
| 227 | Isofenphos-methyl | 甲基异柳磷 | C14H22NO4PS | +Na | 354.08994 | 177.99 | 12.10 | 121.02841 | 109.01096 | 93.03349 |  |  |
| 228 | Isofenphos-oxon | 牛津郡异柳磷 | C15H24NO5P | +Na | 352.12843 | 181.55 | 11.04 | 200.99474 | 121.02841 | 138.99434 | 182.98417 | 200.01072 |
| 229 | Isomethiozin | 丁嗪草酮 | C12H20N4OS | +H | 269.14306 | 165.46 | 12.55 | 172.09029 | 200.08521 | 156.05899 | 142.04334 | 116.02769 |
| 230 | Isonoruron | 异草完隆 | C13H22N2O | +H | 223.18049 | 155.49 | 10.11 | 72.04439 | 91.05423 | 135.11683 | 89.07094 | 107.08553 |
| 231 | Isopropalin | 异丙乐灵 | C15H23N3O4 | +H | 310.17613 | 171.49 | 16.12 | 234.12370 | 208.07167 | 222.08732 | 218.09240 |  |
| 232 | Isoprothiolane | 稻瘟灵 | C12H18O4S2 | +Na | 313.05387 | 175.11 | 10.68 | 188.96746 | 144.97763 | 172.97255 | 84.97426 |  |
| 233 | Isoproturon | 异丙隆 | C12H18N2O | +H | 207.14919 | 150.45 | 8.55 | 72.04439 | 134.09643 | 119.07295 | 118.06513 | 165.10224 |
| 234 | Isopyrazam | 吡唑萘菌胺 | C20H23F2N3O | +H | 360.18820 | 183.70 | 13.28 | 320.17574 | 250.09749 | 238.09749 | 278.12879 | 244.08807 |
| 235 | Isoxaben | 异恶酰草胺 | C18H24N2O4 | +H | 333.18088 | 185.79 | 10.56 | 165.05462 | 150.03115 | 107.01276 | 122.03623 |  |
| 236 | Isoxadifen-ethyl | 双苯恶唑酸 | C18H17NO3 | +Na | 318.11006 | 188.12 | 12.02 | 204.08078 | 203.07027 | 232.07569 | 178.07770 | 250.08626 |
| 237 | Isoxathion | 恶唑磷 | C13H16NO4PS | +H | 314.06104 | 167.01 | 12.73 | 96.95076 | 77.03858 | 162.05495 | 114.96133 | 286.02974 |
| 238 | Ivermectin B1a | 伊维菌素 | C48H74O14 | +Na | 897.49708 | 300.85 | 18.59 | 551.33672 | 307.22677 | 567.33163 |  |  |
| 239 | Kadethrin | 噻嗯菊酯 | C23H24O4S | +H | 397.14681 | 193.51 | 13.60 | 128.06205 | 143.08553 | 91.05423 | 171.08044 |  |
| 240 | Karbutilate | 特胺灵 | C14H21N3O3 | +H | 280.16557 | 171.87 | 6.74 | 181.09715 | 136.03930 | 224.10297 | 72.04439 |  |
| 241 | Kresoxim-methyl | 亚胺菌 | C18H19NO4 | +Na | 336.12063 | 170.97 | 12.12 | 222.09134 | 235.07536 | 206.06004 | 116.04948 | 223.09917 |
| 242 | Lactofen | 乳氟禾草灵 | C19H15ClF3NO7 | +Na | 484.03814 | 211.38 | 14.21 | 222.97682 | 300.00337 | 343.99320 | 178.98699 |  |
| 243 | Leptophos | 溴苯磷 | C13H10BrCl2O2PS | +H | 410.87723 | 169.96 | 16.95 | 171.00280 | 138.97658 | 378.85102 | 155.02564 |  |
| 244 | Linuron | 利谷隆 | C9H10Cl2N2O2 | +H | 249.01921 | 148.91 | 10.19 | 160.97936 | 182.02414 | 125.00268 | 181.01632 | 153.02140 |
| 245 | Malaoxon | 马拉氧磷 | C10H19O7PS | +H | 315.06619 | 162.10 | 6.79 | 124.98206 | 99.00767 | 127.03897 | 142.99263 | 269.02432 |
| 246 | Malathion | 马拉硫磷 | C10H19O6PS2 | +Na | 353.02529 | 171.13 | 10.67 | 124.98206 | 99.00767 | 78.99434 | 127.03897 | 285.00148 |
| 247 | Mandipropamid | 双炔酰菌胺 | C23H22ClNO4 | +H | 412.13101 | 194.84 | 10.46 | 125.01525 | 328.10988 | 164.07061 | 356.10480 |  |
| 248 | Mefenpyr-diethyl | 吡唑解草酯 | C16H18Cl2N2O4 | +H | 373.07164 | 183.51 | 12.65 | 327.02977 | 298.99847 | 252.99299 | 159.97153 |  |
| 249 | Mepanipyrim | 嘧菌胺 | C14H13N3 | +H | 224.11822 | 152.12 | 11.25 | 131.06037 | 77.03858 | 104.04948 | 121.07602 | 106.06513 |
| 250 | Mephospholan | 地胺磷 | C8H16NO3PS2 | +H | 270.03820 | 152.15 | 6.61 | 139.95658 | 167.98788 | 121.94601 | 196.01918 | 242.00690 |
| 251 | Mepronil | 灭锈胺 | C17H19NO2 | +H | 270.14886 | 168.48 | 10.79 | 91.05423 | 228.10191 | 119.04914 | 136.03930 |  |
| 252 | Mesosulfuron-methyl | 甲基二磺隆 | C17H21N5O9S2 | +H | 504.08535 | 199.91 | 7.82 | 182.05602 | 139.05020 | 306.01005 | 162.05495 | 370.99888 |
| 253 | Metaflumizone | 氰氟虫腙 | C24H16F6N4O2 | +H | 507.12502 | 212.70 | 14.25 | 287.07906 | 178.04742 | 267.07283 | 247.06660 | 330.08487 |
| 254 | Metalaxyl | 甲霜灵 | C15H21NO4 | +H | 280.15433 | 160.37 | 8.42 | 160.11208 | 130.06513 | 192.13829 | 248.12812 | 220.13321 |
| 255 | Metamitron | 苯噻草酮 | C10H10N4O | +H | 203.09274 | 141.04 | 5.68 | 175.09782 | 104.04948 | 77.03858 |  |  |
| 256 | Metazachlor | 吡唑草胺 | C14H16ClN3O | +H | 278.10547 | 157.79 | 8.22 | 134.09643 | 105.06988 | 210.06802 |  |  |
| 257 | Metconazole | 叶菌唑 | C17H22ClN3O | +H | 320.15242 | 167.06 | 12.86 | 70.03997 | 125.01525 |  |  |  |
| 258 | Methabenzthiazuron | 甲苯噻隆 | C10H11N3OS | +H | 222.06956 | 141.26 | 8.35 | 165.04810 | 124.02155 | 150.02462 |  |  |
| 259 | Methidathion | 杀扑磷 | C6H11N2O4PS3 | +Na | 324.95108 | 160.20 | 8.99 | 85.03964 | 145.00662 |  |  |  |
| 260 | Methoprene | 烯虫酯 | C19H34O3 | +Na | 333.24002 | 188.90 | 17.06 | 107.08553 | 121.10118 | 191.17943 | 135.11683 |  |
| 261 | Methoprotryne | 盖草津 | C11H21N5OS | +H | 272.15396 | 166.54 | 9.55 | 170.04949 | 198.08079 | 240.12774 | 212.09644 | 230.10701 |
| 262 | Methoxyfenozide | 甲氧虫酰肼 | C22H28N2O3 | +Na | 391.19921 | 202.86 | 10.72 | 149.05971 | 91.05423 | 219.14919 | 313.15467 |  |
| 263 | Metobromuron | 溴谷隆 | C9H11BrN2O2 | +H | 259.00767 | 144.69 | 8.16 | 170.96781 | 169.95999 | 91.04165 | 148.06311 | 147.05529 |
| 264 | Metosulam | 磺草胺唑 | C14H13Cl2N5O4S | +H | 418.01381 | 187.72 | 6.78 | 174.99501 | 140.02615 | 173.98718 |  |  |
| 265 | Metoxuron | 甲氧隆 | C10H13ClN2O2 | +H | 229.07383 | 149.32 | 6.19 | 156.02107 | 106.02874 | 72.04439 |  |  |
| 266 | Metrafenone | 苯菌酮 | C19H21BrO5 | +H | 409.06451 | 181.74 | 13.05 | 209.08084 | 226.97022 | 166.06245 | 165.05462 | 168.96474 |
| 267 | Metribuzin | 草克净 | C8H14N4OS | +H | 215.09611 | 146.34 | 7.09 | 187.10119 | 171.05866 | 131.03859 | 145.05424 | 184.05391 |
| 268 | Metsulfuron-methyl | 甲磺隆 | C14H15N5O6S | +H | 382.08158 | 184.02 | 6.53 | 167.05635 | 263.99478 | 135.04406 | 199.00596 |  |
| 269 | Monalide | 庚酰草胺 | C13H18ClNO | +H | 240.11497 | 156.53 | 11.65 | 93.05730 | 128.02615 |  |  |  |
| 270 | Monolinuron | 绿谷隆 | C9H11ClN2O2 | +H | 215.05818 | 143.01 | 7.66 | 148.06311 | 127.01833 | 98.99960 |  |  |
| 271 | Monuron | 灭草隆 | C9H11ClN2O | +H | 199.06327 | 140.96 | 6.81 | 72.04439 | 126.01050 | 98.99960 |  |  |
| 272 | Moxidectin | 莫昔克丁 | C37H53NO8 | +Na | 662.36634 | 258.38 | 17.76 | 163.06278 | 622.37383 | 441.29994 | 590.34761 |  |
| 273 | Myclobutanil | 腈菌唑 | C15H17ClN4 | +H | 289.12145 | 171.11 | 10.92 | 125.01525 | 70.03997 | 115.05423 | 151.03090 |  |
| 274 | Napropamide | 敌草胺 | C17H21NO2 | +H | 272.16451 | 163.17 | 11.44 | 128.06205 | 171.08044 | 127.05423 | 199.07536 |  |
| 275 | N-desethyl-pirimiphos-methyl | N-去乙基甲基嘧啶磷 | C9H16N3O3PS | +H | 278.07228 | 159.62 | 8.83 | 246.04606 | 218.01476 | 109.00491 | 136.08692 | 124.98206 |
| 276 | Neburon | 草不隆 | C12H16Cl2N2O | +H | 275.07125 | 163.42 | 12.06 | 159.97153 | 88.11208 | 127.01833 | 125.00268 | 132.96063 |
| 277 | Nitenpyram | 烯啶虫胺 | C11H15ClN4O2 | +H | 271.09563 | 160.86 | 4.67 | 160.08692 | 224.09490 | 188.11822 | 126.01050 | 225.10273 |
| 278 | Nitralin | 甲磺乐灵 | C13H19N3O6S | +H | 346.10673 | 177.69 | 11.85 | 262.01283 | 258.01792 | 242.02300 | 304.05978 | 244.00227 |
| 279 | Norflurazon | 氟草敏 | C12H9ClF3N3O | +H | 304.04590 | 159.89 | 8.77 | 284.03967 | 264.03344 | 140.03063 | 145.02596 |  |
| 280 | Nuarimol | 氟苯嘧啶醇 | C17H12ClFN2O | +H | 315.06950 | 168.72 | 10.07 | 252.08192 | 217.02148 | 261.08225 | 138.99452 |  |
| 281 | O,S-TEPP | 硫代-四乙基焦磷酸酯 | C8H20O6P2S | +H | 307.05286 | 156.28 | 9.18 | 80.97361 | 98.98417 | 96.95076 | 194.92766 | 250.99026 |
| 282 | Octhilinone | 辛噻酮 | C11H19NOS | +H | 214.12601 | 156.13 | 11.44 | 102.00081 |  |  |  |  |
| 283 | Ofurace | 呋酰胺 | C14H16ClNO3 | +H | 282.08915 | 154.16 | 6.86 | 144.08078 | 160.11208 | 130.06513 | 148.11208 | 236.08367 |
| 284 | Orbencarb | 坪草丹 | C12H16ClNOS | +H | 258.07139 | 151.46 | 12.90 | 100.07569 | 125.01525 | 89.03858 |  |  |
| 285 | Oryzalin | 黄草消，氨磺乐灵 | C12H18N4O6S | +H | 347.10198 | 176.02 | 11.50 | 198.01455 | 213.02026 | 243.01825 | 259.01317 | 288.02848 |
| 286 | Oxasulfuron | 环丙氧磺隆(环氧嘧磺隆) | C17H18N4O6S | +H | 407.10198 | 197.16 | 6.35 | 150.06619 | 107.06037 | 209.98555 | 184.99031 | 121.02841 |
| 287 | Oxaziclomefone | 噁嗪草酮 | C20H19Cl2NO2 | +H | 376.08656 | 186.99 | 13.99 | 161.05971 | 190.08626 | 133.06479 | 115.05423 |  |
| 288 | Paclobutrazol | 多效唑 | C15H20ClN3O | +H | 294.13677 | 168.17 | 10.64 | 70.03997 | 125.01525 |  |  |  |
| 289 | Paraoxon-ethyl | 乙基对氧磷 | C10H14NO6P | +H | 276.06315 | 157.75 | 7.93 | 174.00765 | 202.99781 | 220.00055 | 94.04132 | 248.03185 |
| 290 | Paraoxon-methyl | 甲基对氧磷 | C8H10NO6P | +H | 248.03185 | 148.47 | 6.25 | 202.03895 | 186.00765 | 231.02911 | 109.00491 | 127.01547 |
| 291 | Penconazole | 戊菌唑 | C13H15Cl2N3 | +H | 284.07158 | 163.39 | 12.27 | 158.97628 | 137.01525 | 172.99193 |  |  |
| 292 | Pencycuron | 戊菌隆 | C19H21ClN2O | +H | 329.14152 | 179.59 | 13.11 | 125.01525 | 89.03858 |  |  |  |
| 293 | Penflufen | 氟唑菌苯胺 | C18H24FN3O | +H | 318.19762 | 175.64 | 12.09 | 141.04587 | 234.10372 | 115.06660 |  |  |
| 294 | Penoxsulam | 五氟磺草胺 | C16H14F5N5O5S | +H | 484.07086 | 194.71 | 7.08 | 194.06725 | 444.05840 | 164.05669 | 166.07234 |  |
| 295 | Pentanochlor | 蔬草灭 | C13H18ClNO | +H | 240.11497 | 156.40 | 12.01 | 106.06513 | 107.07295 | 142.04180 |  |  |
| 296 | Penthiopyrad | 吡噻菌胺 | C16H20F3N3OS | +H | 360.13519 | 177.49 | 12.14 | 177.02702 | 256.03507 | 216.02261 | 276.04129 | 236.02884 |
| 297 | Permethrin,cis | 氯菊酯 | C21H20Cl2O3 | +Na | 413.06817 | 190.96 | 16.94 | 183.08044 | 168.05697 | 319.13287 |  |  |
| 298 | Permethrin,trans | 氯菊酯 | C21H20Cl2O3 | +Na | 413.06817 | 184.88 | 17.44 | 183.08044 | 168.05697 | 319.13287 |  |  |
| 299 | Pethoxamid | 烯草胺 | C14H16ClNO | +H | 250.09932 | 153.83 | 11.39 | 131.08553 | 115.05423 | 216.13829 | 220.16959 |  |
| 300 | Phorate-sulfone | 甲拌磷砜 | C7H17O4PS3 | +Na | 314.99188 | 159.66 | 8.06 | 96.95076 | 114.96133 | 142.93848 | 78.94020 | 171.02393 |
| 301 | Phosfolan | 硫环磷 | C7H14NO3PS2 | +H | 256.02255 | 148.33 | 6.05 | 139.95658 | 121.94601 | 199.95995 | 227.99125 | 167.98788 |
| 302 | Phosfolan-methyl | 甲基硫环磷 | C5H10NO3PS2 | +H | 227.99125 | 138.29 | 5.06 | 167.98788 | 109.00491 | 135.96166 |  |  |
| 303 | Phosphamidon | 磷胺 | C10H19ClNO5P | +H | 300.07621 | 156.64 | 6.18 | 109.00491 | 127.01547 | 174.06802 | 226.98706 |  |
| 304 | Phthalicacid,benzylbutylester | 邻苯二甲酸丁苄酯 | C19H20O4 | +Na | 335.12538 | 177.57 | 13.57 | 91.05423 | 149.02332 | 77.03858 | 121.02841 | 163.03897 |
| 305 | Picolinafen | 氟吡酰草胺 | C19H12F4N2O2 | +H | 377.09077 | 186.96 | 14.37 | 238.04742 | 359.08020 | 145.02596 |  |  |
| 306 | Picoxystrobin | 啶氧菌酯 | C18H16F3NO4 | +Na | 390.09236 | 177.90 | 11.75 | 115.05423 | 145.06479 | 117.06988 | 102.04640 | 177.09101 |
| 307 | Piperalin | 哌丙灵 | C16H21Cl2NO2 | +H | 330.10221 | 176.06 | 7.47 | 172.95555 | 144.96063 | 230.99741 | 140.14338 | 112.11208 |
| 308 | Piperonyl butoxide | 胡椒基丁醚 | C19H30O5 | +Na | 361.19854 | 180.53 | 14.67 | 149.05971 | 177.09101 | 147.08044 |  |  |
| 309 | Piperophos | 哌草磷 | C14H28NO3PS2 | +H | 354.13210 | 181.96 | 13.37 | 142.93848 | 170.93340 | 174.09471 | 252.02763 | 96.95076 |
| 310 | Pirimicarb | 抗蚜威 | C11H18N4O2 | +H | 239.15025 | 154.59 | 7.37 | 182.12879 | 72.04439 | 150.10257 |  |  |
| 311 | Pirimiphos-ethyl | 乙基嘧啶磷 | C13H24N3O3PS | +H | 334.13488 | 176.37 | 14.52 | 198.10594 | 170.07464 | 182.12879 | 154.09749 | 164.11822 |
| 312 | Pirimiphos-methyl | 甲基嘧啶磷 | C11H20N3O3PS | +H | 306.10358 | 166.26 | 12.94 | 278.07228 | 164.11822 | 146.04606 | 108.05562 | 274.07736 |
| 313 | Pretilachlor | 丙草胺 | C14H19ClNO | -e | 252.11497 | 152.55 | 13.76 | 176.14338 | 132.08078 | 147.10425 | 117.05730 | 160.11208 |
| 314 | Primisulfuron-methyl | 氟嘧磺隆 | C15H12F4N4O7S | +H | 469.04356 | 198.84 | 10.66 | 204.02152 | 254.01833 | 186.01096 | 135.04406 |  |
| 315 | Probenazole | 烯丙苯噻唑 | C10H9NO3S | +H | 224.03759 | 139.75 | 6.42 | 168.99539 | 196.00629 | 77.03858 | 165.99573 | 184.00629 |
| 316 | Prochloraz | 咪酰胺 | C15H16Cl3N3O2 | +H | 376.03809 | 181.63 | 12.79 | 308.00064 | 194.91657 | 222.94787 |  |  |
| 317 | Prodiamine | 氨氟乐灵 | C13H17F3N4O4 | +H | 351.12747 | 168.45 | 14.63 | 250.03083 | 232.02026 | 267.03357 | 291.06995 | 309.08052 |
| 318 | Profenofos | 丙溴磷 | C11H15BrClO3PS | +H | 372.94242 | 165.79 | 14.07 | 302.86417 | 128.00234 | 205.93527 | 284.85360 |  |
| 319 | Profoxydim | 环苯草酮 | C24H32ClNO4S | +H | 466.18133 | 209.78 | 16.25 | 280.13658 | 180.10191 | 132.04439 | 194.06341 | 163.07536 |
| 320 | Prometon | 扑灭通 | C10H19N5O | +H | 226.16624 | 156.83 | 8.68 | 142.07234 | 184.11928 | 86.03489 | 100.05054 |  |
| 321 | Prometryn | 扑草净 | C10H19N5S | +H | 242.14339 | 160.24 | 11.04 | 158.04949 | 200.09644 | 116.02769 |  |  |
| 322 | Propachlor | 毒草胺 | C11H14ClNO | +H | 212.08367 | 141.83 | 8.45 | 170.03672 | 94.06513 | 106.06513 | 77.03858 |  |
| 323 | Propamocarb | 霜毒威 | C9H20N2O2 | +H | 189.15975 | 143.97 | 4.33 | 102.05495 | 74.02365 | 144.10191 |  |  |
| 324 | Propanil | 敌稗 | C9H9Cl2NO | +H | 218.01340 | 143.52 | 10.37 | 127.01833 | 161.98718 |  |  |  |
| 325 | Propaphos | 丙虫磷 | C13H21O4PS | +H | 305.09709 | 171.05 | 12.21 | 221.00319 | 202.99263 | 141.03686 | 187.96915 |  |
| 326 | Propaquizafop | 恶草酸 | C22H22ClN3O5 | +H | 444.13207 | 198.37 | 14.45 | 299.05818 | 327.05310 | 255.03197 | 163.00575 | 100.07569 |
| 327 | Propargite | 炔螨特 | C19H26O4S | +Na | 373.14440 | 190.51 | 15.43 | 175.11174 | 81.06988 | 163.11174 | 107.04914 | 231.17434 |
| 328 | Propazine | 扑灭津 | C9H16ClN5 | +H | 230.11670 | 154.72 | 10.16 | 146.02280 | 188.06975 | 104.00100 | 110.04612 | 79.00575 |
| 329 | Propiconazole | 丙环唑 | C15H17Cl2N3O2 | +H | 342.07706 | 176.42 | 12.59 | 158.97628 |  |  |  |  |
| 330 | Propoxycarbazone | 丙苯磺隆 | C15H18N4O7S | +H | 399.09690 | 188.90 | 6.06 | 116.04545 | 199.00596 | 209.98555 | 135.04406 | 367.07068 |
| 331 | Propyzamide | 炔苯烯草胺 | C12H11Cl2NO | +H | 256.02905 | 156.59 | 10.86 | 144.96063 | 172.95555 | 108.98395 | 189.98210 | 110.99960 |
| 332 | Proquinazid | 丙氧喹啉 | C14H17IN2O2 | +H | 373.04075 | 167.81 | 16.28 | 271.92030 | 288.94685 | 330.99380 |  |  |
| 333 | Prosulfocarb | 苄草丹 | C14H21NOS | +H | 252.14166 | 157.51 | 13.87 | 91.05423 |  |  |  |  |
| 334 | Prosulfuron | 氟磺隆 | C15H16F3N5O4S | +H | 420.09479 | 185.89 | 9.85 | 167.05635 | 141.07709 | 109.04480 |  |  |
| 335 | Prothiophos | 丙硫磷 | C11H15Cl2O2PS2 | +H | 344.97009 | 166.36 | 16.76 | 204.92744 | 240.90412 | 160.95555 | 222.89355 |  |
| 336 | Pymetrozine | 吡蚜酮 | C10H11N5O | +H | 218.10364 | 151.62 | 4.33 | 105.04472 | 78.03383 |  |  |  |
| 337 | Pyracarbolid | 吡喃灵 | C13H15NO2 | +H | 218.11756 | 148.26 | 7.15 | 125.05971 | 107.04914 | 97.02841 |  |  |
| 338 | Pyraclofos | 吡唑硫磷 | C14H18ClN2O3PS | +H | 361.05370 | 187.37 | 12.84 | 256.98773 | 138.01050 | 238.97717 | 272.96489 | 195.03197 |
| 339 | Pyraclostrobin | 吡唑醚菊酯 | C19H18ClN3O4 | +H | 388.10586 | 183.58 | 12.70 | 133.05222 | 163.06278 | 149.04713 | 194.08117 | 162.05495 |
| 340 | Pyraflufen-ethyl | 吡草醚 | C15H13Cl2F3N2O4 | +H | 413.02772 | 185.92 | 12.31 | 253.01746 | 338.99094 | 260.99922 | 288.99414 | 304.02209 |
| 341 | Pyrasulfotole | 磺酰草吡唑 | C14H13F3N2O4S | +H | 363.06209 | 174.71 | 5.96 | 250.99843 | 172.01305 | 113.07094 | 144.01814 |  |
| 342 | Pyrazophos | 定菌磷(吡嘧磷 吡菌磷) | C14H20N3O5PS | +H | 374.09340 | 189.68 | 12.96 | 194.05602 | 176.04545 | 222.08732 | 148.05054 | 205.08458 |
| 343 | Pyrazosulfuron-ethyl | 吡嘧磺隆 | C14H18N6O7S | +H | 415.10304 | 192.88 | 11.17 | 182.05602 | 139.05020 | 188.01244 | 213.99170 |  |
| 344 | Pyrazoxyfen | 苄草唑 | C20H16Cl2N2O3 | +H | 403.06107 | 189.34 | 12.34 | 91.05423 | 139.05020 | 172.95555 | 249.04253 | 105.03349 |
| 345 | Pyributicarb | 稗草畏 | C18H22N2O2S | +H | 331.14748 | 186.30 | 14.83 | 108.04439 | 181.04301 | 190.12264 | 93.02092 | 133.10118 |
| 346 | Pyridaben | 哒螨灵 | C19H25ClN2OS | +H | 365.14489 | 193.56 | 16.44 | 147.11683 | 309.08229 | 132.09335 |  |  |
| 347 | Pyridalyl | 啶虫丙醚 | C18H14Cl4F3NO3 | +H | 489.97527 | 201.58 | 18.54 | 164.03177 | 204.06308 | 146.02121 | 183.02073 | 108.96063 |
| 348 | Pyridaphenthion | 哒嗪硫磷 | C14H17N2O4PS | +H | 341.07194 | 174.28 | 10.90 | 189.06585 | 205.04301 | 171.05529 | 92.04948 |  |
| 349 | Pyrifenox-1 | 啶斑亏 | C14H12Cl2N2O | +H | 295.03994 | 167.25 | 11.03 | 93.05730 | 92.04948 | 263.01373 |  |  |
|  | Pyrifenox-2 | 啶斑亏 | C14H12Cl2N2O | +H | 295.03994 | 166.54 | 11.45 | 93.05730 | 92.04948 | 263.01373 |  |  |
| 350 | Pyriftalid | 环酯草醚 | C15H14N2O4S | +H | 319.07470 | 165.81 | 9.49 | 179.01613 | 301.06414 | 273.06922 | 287.04849 | 139.05020 |
| 351 | Pyrimethanil | 嘧霉胺 | C12H13N3 | +H | 200.11822 | 142.82 | 10.09 | 183.09167 | 107.06037 |  |  |  |
| 352 | Pyriproxyfen | 吡丙醚 | C20H19NO3 | +H | 322.14377 | 182.80 | 14.84 | 78.03383 | 185.05971 | 96.04439 | 227.10666 |  |
| 353 | Pyrithiobac | 嘧草硫醚 | C13H11ClN2O4S | +H | 327.02008 | 165.21 | 8.25 | 309.00952 | 199.99314 | 139.05020 | 195.96184 |  |
| 354 | Pyroquilon | 咯喹酮 | C11H11NO | +H | 174.09134 | 134.91 | 6.80 | 117.05730 | 132.08078 |  |  |  |
| 355 | Pyroxasulfone | 砜吡草唑 | C12H14F5N3O4S | +H | 392.06979 | 177.11 | 7.91 | 179.04267 | 159.03645 | 229.03948 | 131.04153 |  |
| 356 | Pyroxsulam | 啶磺草胺 | C14H13F3N6O5S | +H | 435.06930 | 187.39 | 6.55 | 194.06725 | 166.07234 | 124.05054 | 152.04545 | 258.02915 |
| 357 | Quinalphos | 喹硫磷 | C12H15N2O3PS | +H | 299.06138 | 161.80 | 12.07 | 163.03245 | 129.04472 | 147.05529 | 242.99878 | 96.95076 |
| 358 | Quinoclamine | 灭藻醌 | C10H6ClNO2 | +H | 208.01598 | 133.17 | 6.67 | 172.03930 | 77.03858 | 144.04439 | 137.01525 | 105.03349 |
| 359 | Quinoxyfen | 苯氧喹啉 | C15H8Cl2FNO | +H | 308.00397 | 161.26 | 15.06 | 272.02730 | 162.01050 | 196.97936 | 213.98210 | 287.99775 |
| 360 | Quizalofop-ethyl | 喹禾灵 | C19H17ClN2O4 | +H | 373.09496 | 191.95 | 14.12 | 299.05818 | 255.03197 | 163.00575 | 244.03979 |  |
| 361 | Rabenzazole | 吡咪唑 | C12H12N4 | +H | 213.11347 | 145.59 | 8.45 | 172.08692 | 118.05255 |  |  |  |
| 362 | Resmethrin | 灭虫菊酯 | C22H26O3 | +H | 339.19547 | 184.53 | 16.82 | 91.05423 | 171.08044 | 77.03858 |  |  |
| 363 | Rimsulfuron | 玉嘧磺隆(砜嘧磺隆) | C14H17N5O7S2 | +H | 432.06422 | 193.33 | 7.16 | 182.05602 | 325.09650 | 139.05020 | 106.06513 |  |
| 364 | Rotenone | 鱼藤酮 | C23H22O6 | +H | 395.14891 | 196.02 | 11.77 | 191.07027 | 213.09101 | 198.06753 | 203.07027 | 177.05462 |
| 365 | Saflufenacil | 苯嘧磺草胺 | C17H17ClF4N4O5S | +H | 501.06171 | 207.89 | 9.30 | 348.99976 | 197.97526 | 459.01476 | 366.02631 | 141.98543 |
| 366 | Sebuthylazine | 另丁津 | C9H16ClN5 | +H | 230.11670 | 152.67 | 9.99 | 174.05410 | 104.00100 | 146.02280 | 68.02432 | 132.03230 |
| 367 | Sebuthylazine-desethyl | 脱乙基另丁津 | C7H12ClN5 | +H | 202.08540 | 143.91 | 6.72 | 146.02280 | 104.00100 | 110.04612 |  |  |
| 368 | Secbumeton | 密草通 | C10H19N5O | +H | 226.16624 | 155.20 | 8.59 | 170.10364 | 142.07234 | 114.06619 |  |  |
| 369 | Sethoxydim | 稀禾定 | C17H29NO3S | +H | 328.19409 | 181.92 | 14.39 | 178.08626 | 180.10191 | 161.05971 | 150.09134 | 220.13321 |
| 370 | Siduron | 环草隆 | C14H20N2O | +H | 233.16484 | 156.44 | 10.22 | 77.03858 | 137.07094 | 94.06513 | 120.04439 |  |
| 371 | Silthiofam | 硅噻菌胺 | C13H21NOSSi | +H | 268.11859 | 161.31 | 11.96 | 252.08729 | 197.04509 | 210.04034 | 139.02121 |  |
| 372 | Simazine | 西玛津 | C7H12ClN5 | +H | 202.08540 | 141.79 | 7.04 | 174.05410 | 104.00100 | 68.02432 | 132.03230 | 124.08692 |
| 373 | Simeconazole | 硅氟唑 | C14H20FN3OSi | +H | 294.14324 | 166.89 | 11.37 | 115.05423 | 133.04480 | 70.03997 | 135.06045 |  |
| 374 | Simeton | 西玛通/西马津 | C8H15N5O | +H | 198.13494 | 143.90 | 6.27 | 100.05054 | 68.02432 | 128.08184 | 170.10364 | 124.08692 |
| 375 | Simetryn | 西草净 | C8H15N5S | +H | 214.11209 | 148.45 | 7.88 | 124.08692 | 144.05899 | 166.10872 | 116.02769 | 96.05562 |
| 376 | S-Metolachlor | S-异丙甲草胺 | C15H22ClNO2 | +H | 284.14118 | 158.70 | 11.62 | 176.14338 | 252.11497 | 134.09643 | 146.09643 | 160.11208 |
| 377 | Spinetoram | 乙基多杀菌素 | C42H69NO10 | +H | 748.49942 | 276.78 | 13.59 | 142.12264 | 98.09643 |  |  |  |
| 378 | Spinosad A/D | 多杀霉素 A | C41H65NO10 | +H | 732.46812 | 272.07 | 12.81 | 142.12264 | 98.09643 |  |  |  |
| 379 | Spirokamine | 螺咯胺 | C18H35NO2 | +H | 298.27406 | 180.85 | 10.43 | 144.13829 | 100.11208 | 72.08078 |  |  |
| 380 | Spiromesifen | 螺甲螨酯 | C23H30O4 | +Na | 393.20363 | 201.92 | 15.23 | 273.14852 | 255.13796 | 187.07536 | 209.13248 |  |
| 381 | Spirotetramat | 螺虫乙酯 | C21H27NO5 | +H | 374.19620 | 190.87 | 11.20 | 216.10191 | 270.14886 | 244.13321 | 330.20637 | 302.17507 |
| 382 | Spiroxamine | 螺环菌胺 | C18H35NO2 | +H | 298.27406 | 179.15 | 10.17 | 144.13829 | 100.11208 | 72.08078 |  |  |
| 383 | Sulcotrione | 磺草酮 | C14H13ClO5S | +H | 329.02450 | 170.69 | 5.95 | 293.04782 | 68.99711 | 249.03130 | 111.04406 | 139.03897 |
| 384 | Sulfentrazone | 甲磺草胺 | C11H10Cl2F2N4O3S | +Na | 408.97109 | 181.25 | 7.06 | 273.03492 | 306.99595 | 182.01157 | 198.94604 | 279.98505 |
| 385 | Sulfometuron-methyl | 甲嘧磺隆 | C15H16N4O5S | +H | 365.09142 | 184.00 | 6.70 | 150.06619 | 107.06037 | 135.04406 |  |  |
| 386 | Sulfosulfuron | 磺酰磺隆 | C16H18N6O7S2 | +H | 471.07511 | 199.51 | 9.40 | 211.05357 | 261.02882 | 139.03763 | 156.07675 |  |
| 387 | Sulfotep | 治螟磷 | C8H20O5P2S2 | +H | 323.03001 | 158.82 | 12.13 | 96.95076 | 114.96133 | 142.99263 | 266.96741 | 171.02393 |
| 388 | Sulprofos | 甲丙硫磷 | C12H19O2PS3 | +H | 323.03575 | 169.49 | 15.17 | 154.97150 | 200.95922 | 218.96978 | 139.02121 | 247.00108 |
| 389 | TCMTB | 苯噻硫氰 | C8H6NS2 | -e | 179.99362 | 129.51 | 10.06 | 136.02155 | 109.01065 | 166.98579 | 135.01372 |  |
| 390 | Tebuconazole | 戊唑醇 | C16H22ClN3O | +H | 308.15242 | 165.89 | 12.36 | 70.03997 | 125.01525 |  |  |  |
| 391 | Tebufenpyrad | 吡螨胺 | C18H24ClN3O | +H | 334.16807 | 192.29 | 14.33 | 145.05270 | 117.02140 | 171.03197 | 147.11683 |  |
| 392 | Tebupirimfos | 丁基嘧啶磷 | C13H23N2O3PS | +H | 319.12398 | 176.25 | 14.55 | 153.10224 | 231.03516 | 249.04573 | 215.05801 | 277.07703 |
| 393 | Tebutam | 牧草胺 | C15H23NO | +H | 234.18524 | 154.85 | 11.58 | 91.05423 | 192.13829 |  |  |  |
| 394 | Tebuthiuron | 丁噻隆 | C9H16N4OS | +H | 229.11176 | 150.08 | 7.17 | 172.09029 | 116.02769 | 157.06682 | 142.04334 |  |
| 395 | Tefluthrin | 七氟菊酯 | C17H14ClF7O2 | +NH4 | 436.09088 | 196.27 | 6.22 | 91.05423 | 126.02756 | 134.03623 | 109.02841 | 93.03349 |
| 396 | Temephos | 双硫磷 | C16H20O6P2S3 | +H | 466.99700 | 205.93 | 14.41 | 341.00656 | 418.99363 | 404.97798 |  |  |
| 397 | Tepraloxydim | 快捕净 | C17H24ClNO4 | +H | 342.14666 | 185.19 | 11.16 | 250.14377 | 166.08626 | 149.05971 | 222.14886 | 164.07061 |
| 398 | Terbufos-sulfone | 特丁硫磷砜 | C9H21O4PS3 | +Na | 343.02318 | 170.49 | 9.77 | 96.95076 | 114.96133 | 142.93848 | 78.94020 | 98.94865 |
| 399 | Terbufos-sulfoxide | 特丁硫磷亚砜 | C9H21O3PS3 | +Na | 327.02826 | 168.48 | 9.79 | 130.93848 | 96.95076 | 158.96978 | 187.00108 |  |
| 400 | Terbumeton | 特丁通 | C10H19N5O | +H | 226.16624 | 155.61 | 9.01 | 170.10364 | 142.07234 | 114.06619 | 128.08184 | 100.05054 |
| 401 | Terbuthylazine-desethyl | 去乙基特丁津 | C7H12ClN5 | +H | 202.08540 | 143.33 | 7.32 | 146.02280 | 110.04612 | 104.00100 |  |  |
| 402 | Terbutryn | 特丁净(去草净) | C10H19N5S | +H | 242.14339 | 159.56 | 11.19 | 186.08079 | 158.04949 |  |  |  |
| 403 | Tetraconazole | 四氟醚唑 | C13H11Cl2F4N3O | +H | 372.02881 | 174.12 | 11.34 | 157.97628 | 204.03230 | 70.03997 | 336.05213 |  |
| 404 | Tetramethrin | 胺菊酯 | C19H25NO4 | +Na | 354.16758 | 197.86 | 14.28 | 164.07061 | 135.11683 | 314.17507 | 332.18563 | 286.18016 |
| 405 | Thenylchlor | 甲氧噻草胺 | C16H18ClNO2S | +Na | 346.06390 | 178.75 | 11.30 | 134.09643 | 288.10528 | 246.09471 | 127.02121 |  |
| 406 | Thiabendazole | 噻菌灵 | C10H7N3S | +H | 202.04334 | 136.80 | 5.76 | 175.03245 | 131.06037 |  |  |  |
| 407 | Thiabendazole-5-hydroxy | 5-羟基噻苯哒唑 | C10H7N3OS | +H | 218.03826 | 141.06 | 4.91 | 191.02736 | 159.05529 | 108.04439 | 147.05529 |  |
| 408 | Thiacloprid | 噻虫啉 | C10H9ClN4S | +H | 253.03092 | 155.17 | 5.79 | 126.01050 | 90.03383 | 99.00115 |  |  |
| 409 | Thiamethoxam | 噻虫嗪 | C8H10ClN5O3S | +Na | 314.00851 | 158.42 | 4.93 | 181.05424 | 211.06481 | 108.05562 | 152.02769 |  |
| 410 | Thiazopyr | 噻唑烟酸 | C16H17F5N2O2S | +H | 397.10037 | 180.81 | 12.09 | 377.09414 | 335.04719 | 303.02097 | 275.02606 | 297.08454 |
| 411 | Thidiazuron | 噻苯隆 | C9H8N4OS | +H | 221.04916 | 144.69 | 6.95 | 102.01204 | 127.99131 | 77.03858 | 94.06513 |  |
| 412 | Thiencarbazone-methyl | 噻酮磺隆 | C12H14N4O7S2 | +H | 391.03767 | 180.48 | 5.98 | 130.06110 | 229.95763 | 218.97803 | 139.99265 | 283.96685 |
| 413 | Thifensulfuron-methyl | 噻吩磺隆 | C12H13N5O6S2 | +H | 388.03800 | 183.87 | 6.39 | 167.05635 | 204.96238 | 269.95120 | 174.95181 | 125.97700 |
| 414 | Thiodicarb | 硫双威 | C10H18N4O4S3 | +Na | 377.03824 | 190.15 | 7.29 | 88.02155 |  |  |  |  |
| 415 | Thiophanate-ethyl | 硫菌灵 | C14H18N4O4S2 | +H | 371.08422 | 186.25 | 8.66 | 151.03245 | 160.05054 | 118.05255 | 134.07127 | 149.01680 |
| 416 | Thiophanate-methyl | 甲基托布津 | C12H14N4O4S2 | +H | 343.05292 | 173.02 | 6.71 | 151.03245 | 160.05054 | 226.06447 | 268.02089 | 311.02671 |
| 417 | Tolclofos-methyl | 甲基立枯磷 | C9H11Cl2O3PS | +H | 300.96163 | 149.08 | 12.94 | 174.97120 | 218.94309 | 253.91194 | 268.93542 |  |
| 418 | Tolfenpyrad | 唑虫酰胺 | C21H22ClN3O2 | +H | 384.14733 | 206.68 | 14.52 | 197.09609 | 154.07770 | 169.10118 | 171.03197 | 145.05270 |
| 419 | Tralkoxydim | 三甲苯草酮 | C20H27NO3 | +H | 330.20637 | 187.10 | 15.15 | 284.16451 | 138.05495 | 96.04439 |  |  |
| 420 | Triadimefon | 三唑酮 | C14H16ClN3O2 | +H | 294.10038 | 171.92 | 10.83 | 141.01017 | 197.07277 | 129.01017 | 126.99452 |  |
| 421 | Tri-allate | 野麦畏 | C10H16Cl3NOS | +H | 304.00909 | 159.83 | 15.26 | 142.92166 | 82.94498 |  |  |  |
| 422 | Triasulfuron | 醚苯磺隆 | C14H16ClN5O5S | +H | 402.06334 | 186.01 | 6.40 | 167.05635 | 141.07709 | 83.02399 | 183.01104 | 137.00556 |
| 423 | Triazophos | 三唑磷 | C12H16N3O3PS | +H | 314.07228 | 172.11 | 11.04 | 162.06619 | 119.06037 | 96.95076 |  |  |
| 424 | Triazoxide | 咪唑嗪 | C10H6ClN5O | +H | 248.03336 | 148.68 | 8.29 | 149.99793 | 203.02448 | 221.02247 | 123.99485 |  |
| 425 | Tribufos (DEF) | 脱叶磷 | C12H27OPS3 | +H | 315.10344 | 175.96 | 16.47 | 112.92792 | 168.99052 | 259.04084 | 225.05312 |  |
| 426 | Trichlorfon | 敌百虫 | C4H8Cl3O4P | +H | 256.92985 | 135.09 | 5.67 | 109.00491 | 220.95318 | 127.01547 |  |  |
| 427 | Tricyclazole | 三环唑 | C9H7N3S | +H | 190.04334 | 133.78 | 6.04 | 163.03245 | 136.02155 | 121.01065 | 146.00590 |  |
| 428 | Tridemorph | 十三吗啉 | C19H39NO | +H | 298.31044 | 187.38 | 12.58 | 130.12264 | 240.26858 |  |  |  |
| 429 | Trietazine | 草达津 | C9H16ClN5 | +H | 230.11670 | 150.44 | 11.39 | 202.08540 | 174.05410 | 132.03230 | 124.08692 | 104.00100 |
| 430 | Trifloxystrobin | 肟菌酯 | C20H19F3N2O4 | +H | 409.13697 | 188.51 | 13.37 | 186.05251 | 145.02596 | 206.08117 |  |  |
| 431 | Trifloxysulfuron | 三氟啶磺隆 | C14H14F3N5O6S | +H | 438.06896 | 191.17 | 7.97 | 182.05602 | 176.03177 | 139.05020 | 257.02022 |  |
| 432 | Triflumizole | 氟菌唑 | C15H15ClF3N3O | +H | 346.09285 | 177.00 | 13.63 | 178.98699 | 205.99789 | 278.05540 |  |  |
| 433 | Triflumuron | 杀铃脲 | C15H10ClF3N2O3 | +H | 359.04048 | 168.71 | 12.78 | 138.99452 | 110.99960 | 156.02107 |  |  |
| 434 | Triflusulfuron-methyl | 氟胺磺隆 | C17H19F3N6O6S | +H | 493.11116 | 210.17 | 10.43 | 264.07029 | 238.09102 | 96.05562 | 461.08495 |  |
| 435 | Tritosulfuron | 三氟甲磺隆 | C13H9F6N5O4S | +H | 446.03522 | 185.04 | 8.42 | 195.04882 | 145.02596 | 221.02809 | 110.02231 |  |
| 436 | Valifenalate-1 | 缬菌胺 | C19H27ClN2O5 | +H | 399.16813 | 200.09 | 10.74 | 155.02582 | 165.01017 | 197.03638 | 313.13135 |  |
|  | Valifenalate-2 | 缬菌胺 | C19H27ClN2O5 | +H | 399.16813 | 200.57 | 10.96 | 155.02582 | 165.01017 | 197.03638 |  |  |
| 437 | Vernolate | 灭草敌 | C10H21NOS | +H | 204.14166 | 146.71 | 13.23 | 162.09471 | 102.12773 |  |  |  |
| 438 | Zoxamide | 苯酰草胺 | C14H16Cl3NO2 | +H | 336.03194 | 174.44 | 12.66 | 158.97628 | 186.97120 | 122.99960 | 300.05526 |  |

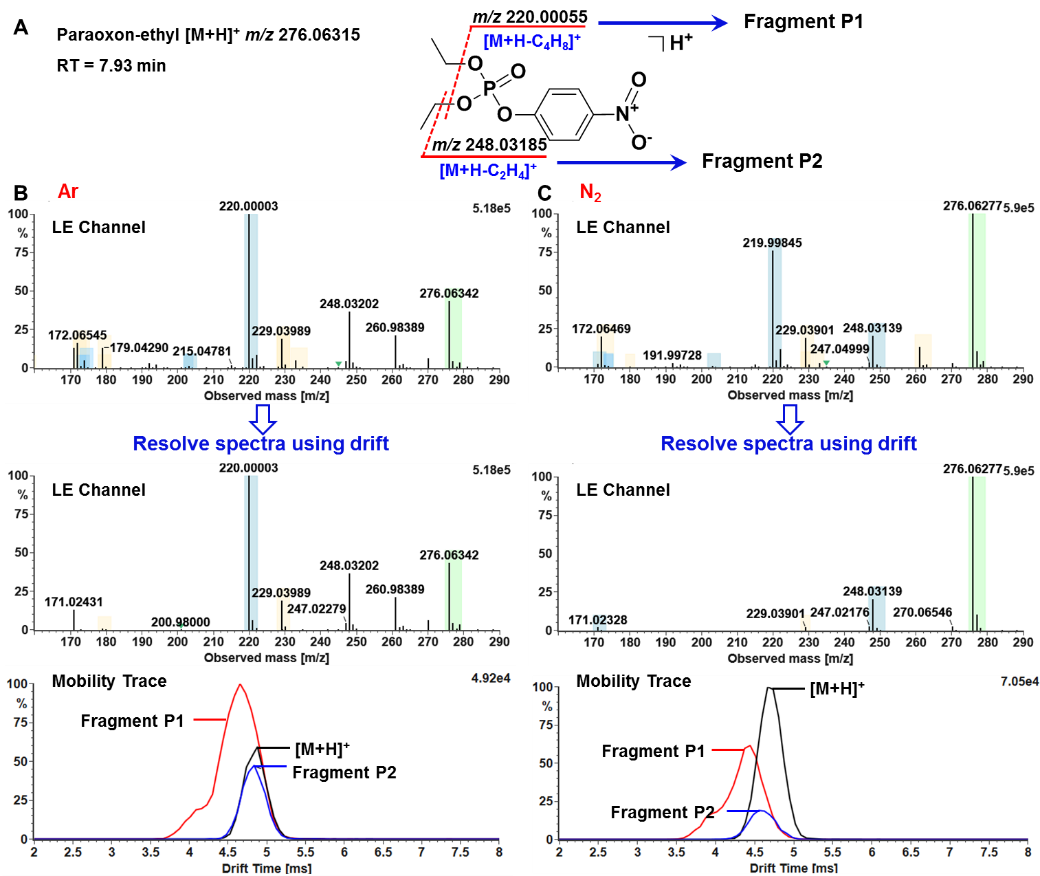
Table S6 Validation results for qualitative analyses of 438 pesticides spiked to the ten LJF samples at three concentration levels.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Item Name | No. of Detections | | | SDL (mg/kg) |
| 0.01 mg/kg | 0.05 mg/kg | 0.20 mg/kg |
| Abamectin-B1a | 0 | 4 | 15 | > 0.2 |
| Acetamiprid | 2 | 15 | 19 | 0.2 |
| Acetochlor | 19 | 20 | 20 | 0.01 |
| Akton | 6 | 20 | 20 | 0.05 |
| Aldicarb-sulfone | 3 | 18 | 19 | 0.2 |
| Alloxydim | 3 | 20 | 20 | 0.05 |
| Ametoctradin | 0 | 0 | 20 | 0.2 |
| Ametryn | 20 | 20 | 20 | 0.01 |
| Amicarbazone | 0 | 9 | 11 | > 0.2 |
| Aminocarb | 4 | 19 | 20 | 0.05 |
| Anilofos | 20 | 20 | 20 | 0.01 |
| Atrazine | 20 | 20 | 20 | 0.01 |
| Atrazine-desethyl | 3 | 5 | 16 | > 0.2 |
| Atrazine-desisopropyl | 18 | 18 | 17 | > 0.2 |
| Azaconazole | 20 | 20 | 20 | 0.01 |
| Azamethiphos | 20 | 20 | 20 | 0.01 |
| Azimsulfuron | 20 | 20 | 20 | 0.01 |
| Azinphos-ethyl | 0 | 10 | 20 | 0.2 |
| Azinphos-methyl | 0 | 0 | 20 | 0.2 |
| Aziprotryne | 19 | 20 | 20 | 0.01 |
| Azoxystrobin | 20 | 20 | 20 | 0.01 |
| Beflubutamid | 20 | 20 | 20 | 0.01 |
| Benalaxyl | 20 | 20 | 20 | 0.01 |
| Benfuracarb | 0 | 4 | 16 | > 0.2 |
| Benodanil | 20 | 20 | 20 | 0.01 |
| Benoxacor | 20 | 20 | 20 | 0.01 |
| Bensulfuron-methyl | 19 | 20 | 20 | 0.01 |
| Bensulide | 0 | 18 | 20 | 0.2 |
| Benthiavalicarb-isopropyl | 20 | 20 | 20 | 0.01 |
| Benzoximate | 0 | 0 | 18 | > 0.2 |
| Benzoylprop-ethyl | 0 | 0 | 18 | > 0.2 |
| Benzyladenine | 15 | 20 | 20 | 0.05 |
| Bispyribac | 20 | 20 | 20 | 0.01 |
| Boscalid | 19 | 20 | 20 | 0.01 |
| Bromfenvinfos | 20 | 20 | 20 | 0.01 |
| Brompyrazon | 4 | 20 | 20 | 0.05 |
| Bromuconazole,cis | 4 | 20 | 20 | 0.05 |
| Bromuconazole,trans | 0 | 19 | 20 | 0.05 |
| Bupirimate | 20 | 20 | 20 | 0.01 |
| Buprofezin | 20 | 20 | 20 | 0.01 |
| Butafenacil | 20 | 20 | 20 | 0.01 |
| Butralin | 0 | 19 | 20 | 0.05 |
| Buturon | 20 | 20 | 20 | 0.01 |
| Cafenstrole | 0 | 17 | 20 | 0.2 |
| Carbetamide | 0 | 2 | 12 | > 0.2 |
| Carbosulfan | 0 | 12 | 17 | > 0.2 |
| Carboxin | 18 | 20 | 20 | 0.05 |
| Carfentrazone-ethyl | 18 | 20 | 20 | 0.05 |
| Carpropamid | 18 | 20 | 20 | 0.05 |
| Chlorantraniliprole | 20 | 20 | 20 | 0.01 |
| Chlorbromuron | 20 | 20 | 20 | 0.01 |
| Chlorfenvinphos | 20 | 20 | 20 | 0.01 |
| Chloridazon | 0 | 20 | 20 | 0.05 |
| Chlorimuron-ethyl | 0 | 20 | 20 | 0.05 |
| Chloroxuron | 20 | 20 | 20 | 0.01 |
| Chlorphoxim | 20 | 20 | 20 | 0.01 |
| Chlorpyrifos | 20 | 20 | 20 | 0.01 |
| Chlorpyrifos-methyl | 0 | 20 | 20 | 0.05 |
| Chlorpyrifos-oxon | 20 | 20 | 20 | 0.01 |
| Chlorsulfuron | 20 | 20 | 20 | 0.01 |
| Chlortoluron | 20 | 20 | 20 | 0.01 |
| Cinidon-ethyl | 0 | 1 | 0 | undetectable |
| Cinosulfuron | 20 | 20 | 20 | 0.01 |
| Clethodim | 0 | 0 | 16 | > 0.2 |
| Clodinafop-propargyl | 20 | 20 | 20 | 0.01 |
| Clomazone | 20 | 20 | 20 | 0.01 |
| Cloransulam-methyl | 20 | 20 | 20 | 0.01 |
| Coumaphos | 20 | 20 | 20 | 0.01 |
| Coumaphos-oxon | 19 | 20 | 20 | 0.01 |
| Coumatetralyl | 20 | 20 | 20 | 0.01 |
| Crimidine | 0 | 20 | 20 | 0.05 |
| Crufomate | 20 | 20 | 20 | 0.01 |
| Cumyluron | 19 | 20 | 20 | 0.01 |
| Cyanazine | 12 | 20 | 20 | 0.05 |
| Cyazofamid | 20 | 20 | 20 | 0.01 |
| Cycluron | 20 | 20 | 20 | 0.01 |
| Cyflufenamid | 20 | 20 | 20 | 0.01 |
| Cyhalothrin | 2 | 12 | 20 | 0.2 |
| Cymiazole | 0 | 0 | 20 | 0.2 |
| Cyprazine | 20 | 20 | 20 | 0.01 |
| Cyproconazole-1 | 18 | 20 | 20 | 0.05 |
| Cyproconazole-2 | 15 | 19 | 20 | 0.05 |
| Cyprodinil | 20 | 20 | 20 | 0.01 |
| Cyprofuram | 0 | 20 | 20 | 0.05 |
| Cyprosulfamide | 18 | 20 | 20 | 0.05 |
| Cythioate | 0 | 6 | 20 | 0.2 |
| DEET | 20 | 20 | 20 | 0.01 |
| Demeton-S-methyl-sulfoxide | 6 | 20 | 20 | 0.05 |
| Demeton-S-methyl-sulphon | 20 | 20 | 20 | 0.01 |
| Desmedipham | 0 | 12 | 20 | 0.2 |
| Diallate | 0 | 5 | 19 | 0.2 |
| Diazinon | 20 | 20 | 20 | 0.01 |
| Diazinon-O-analog | 11 | 20 | 20 | 0.05 |
| Dichlorfenthion | 0 | 0 | 18 | > 0.2 |
| Dichlorvos | 0 | 20 | 20 | 0.05 |
| Diclobutrazol | 20 | 20 | 20 | 0.01 |
| Diclosulam | 18 | 20 | 20 | 0.05 |
| Dicrotophos | 0 | 12 | 20 | 0.2 |
| Diethatyl-ethyl | 20 | 20 | 20 | 0.01 |
| Diethofencarb | 0 | 0 | 20 | 0.2 |
| Difenoconazole | 20 | 20 | 20 | 0.01 |
| Difenoxuron | 20 | 20 | 20 | 0.01 |
| Difenzoquat-methyl-sulfate | 9 | 20 | 19 | 0.05 |
| Diflufenican | 20 | 20 | 20 | 0.01 |
| Dimefuron | 20 | 20 | 20 | 0.01 |
| Dimethachlor | 20 | 20 | 20 | 0.01 |
| Dimethametryn | 20 | 20 | 20 | 0.01 |
| Dimethenamid | 20 | 20 | 20 | 0.01 |
| Dimethomorph-1 | 20 | 20 | 20 | 0.01 |
| Dimethomorph-2 | 19 | 20 | 20 | 0.01 |
| Dimethylvinphos | 20 | 20 | 20 | 0.01 |
| Dimetilan | 2 | 18 | 20 | 0.2 |
| Dimoxystrobin | 1 | 3 | 1 | undetectable |
| Diniconazole | 20 | 20 | 20 | 0.01 |
| Dinitramine | 0 | 19 | 20 | 0.05 |
| Dioxathion-1 | 18 | 20 | 20 | 0.05 |
| Dioxathion-2 | 20 | 20 | 20 | 0.01 |
| Diphenamid | 20 | 20 | 20 | 0.01 |
| Dipropetryn | 0 | 0 | 0 | undetectable |
| Disulfoton sulfone | 20 | 20 | 20 | 0.01 |
| Dithiopyr | 20 | 20 | 20 | 0.01 |
| Diuron | 20 | 20 | 20 | 0.01 |
| Dodemorph | 20 | 20 | 20 | 0.01 |
| Dodine | 3 | 19 | 20 | 0.05 |
| Doramectin | 0 | 0 | 15 | > 0.2 |
| Drazoxolon | 18 | 20 | 20 | 0.05 |
| Edifenphos | 14 | 19 | 20 | 0.05 |
| Emamectin B1A Benzoate | 1 | 5 | 17 | > 0.2 |
| EPN | 1 | 20 | 20 | 0.05 |
| Eprinomectin B1a | 0 | 1 | 14 | > 0.2 |
| Esprocarb | 20 | 20 | 20 | 0.01 |
| Etaconazole | 20 | 20 | 20 | 0.01 |
| Ethametsulfuron-methyl | 10 | 20 | 20 | 0.05 |
| Ethidimuron | 0 | 0 | 19 | 0.2 |
| Ethiprole | 20 | 20 | 20 | 0.01 |
| Ethirimol | 5 | 12 | 20 | 0.2 |
| Ethoprophos | 20 | 20 | 20 | 0.01 |
| Ethoxysulfuron | 19 | 20 | 20 | 0.01 |
| Etobenzanid | 20 | 20 | 20 | 0.01 |
| Etoxazole | 20 | 20 | 20 | 0.01 |
| Famphur | 20 | 20 | 20 | 0.01 |
| Fenamidone | 20 | 20 | 20 | 0.01 |
| Fenamiphos | 18 | 19 | 20 | 0.05 |
| Fenamiphos sulfone | 20 | 20 | 20 | 0.01 |
| Fenamiphos sulfoxide | 20 | 20 | 20 | 0.01 |
| Fenarimol | 19 | 20 | 20 | 0.01 |
| Fenazaquin | 20 | 20 | 20 | 0.01 |
| Fenbuconazole | 20 | 20 | 20 | 0.01 |
| Fenchlorphos oxon | 20 | 20 | 20 | 0.01 |
| Fenfuram | 20 | 20 | 20 | 0.01 |
| Fenhexamid | 18 | 20 | 20 | 0.05 |
| Fenoxaprop-ethyl | 20 | 20 | 20 | 0.01 |
| Fenoxycarb | 20 | 20 | 20 | 0.01 |
| Fenpiclonil | 0 | 20 | 20 | 0.05 |
| Fenpropidin | 20 | 20 | 20 | 0.01 |
| Fenpyrazamine | 20 | 20 | 20 | 0.01 |
| Fenpyroximate | 20 | 20 | 20 | 0.01 |
| Fensulfothion | 20 | 20 | 20 | 0.01 |
| Fensulfothion-oxon | 20 | 20 | 20 | 0.01 |
| Fensulfothion-oxon-sulfone | 15 | 20 | 20 | 0.05 |
| Fensulfothion-sulfone | 20 | 20 | 20 | 0.01 |
| Fenthion | 15 | 20 | 20 | 0.05 |
| Fenthion-oxon-sulfoxide | 0 | 20 | 20 | 0.05 |
| Fenthion-sulfone | 20 | 20 | 20 | 0.01 |
| Fenthion-sulfoxide | 20 | 20 | 20 | 0.01 |
| Ferimzone | 19 | 20 | 20 | 0.01 |
| Fipronil-sulfone | 0 | 0 | 11 | > 0.2 |
| Flamprop-isopropyl | 1 | 20 | 20 | 0.05 |
| Flazasulfuron | 20 | 20 | 20 | 0.01 |
| Flonicamid | 0 | 17 | 20 | 0.2 |
| Florasulam | 0 | 17 | 20 | 0.2 |
| Fluazifop-p-butyl | 20 | 20 | 20 | 0.01 |
| Fluazuron | 20 | 20 | 20 | 0.01 |
| Flubendiamide | 17 | 20 | 20 | 0.05 |
| Flucarbazone | 0 | 0 | 19 | 0.2 |
| Flucycloxuron | 0 | 11 | 20 | 0.2 |
| Flucythrinate | 0 | 20 | 20 | 0.05 |
| Flufenacet | 0 | 0 | 19 | 0.2 |
| Flufenpyr-ethyl | 20 | 20 | 20 | 0.01 |
| Flumetsulam | 0 | 13 | 20 | 0.2 |
| Flumiclorac-pentyl | 20 | 20 | 20 | 0.01 |
| Flumioxazin | 8 | 20 | 20 | 0.05 |
| Fluometuron | 20 | 20 | 20 | 0.01 |
| Fluopicolide | 19 | 20 | 20 | 0.01 |
| Fluopyram | 20 | 20 | 20 | 0.01 |
| Fluoroglycofen-ethyl | 20 | 20 | 20 | 0.01 |
| Fluoxastrobin | 20 | 20 | 20 | 0.01 |
| Fluquinconazole | 3 | 20 | 20 | 0.05 |
| Fluridone | 20 | 20 | 20 | 0.01 |
| Flurochloridone | 17 | 20 | 20 | 0.05 |
| Flurprimidol | 20 | 20 | 20 | 0.01 |
| Flurtamone | 20 | 20 | 20 | 0.01 |
| Flusilazole | 20 | 20 | 20 | 0.01 |
| Fluthiacet-methyl | 20 | 20 | 20 | 0.01 |
| Flutolanil | 20 | 20 | 20 | 0.01 |
| Flutriafol | 20 | 20 | 20 | 0.01 |
| Fluxapyroxad | 20 | 20 | 20 | 0.01 |
| Foramsulfuron | 20 | 20 | 20 | 0.01 |
| Forchlorfenuron | 20 | 20 | 20 | 0.01 |
| Fosthiazate | 20 | 20 | 20 | 0.01 |
| Fuberidazole | 0 | 13 | 19 | 0.2 |
| Furalaxyl | 20 | 20 | 20 | 0.01 |
| Furametpyr | 20 | 20 | 20 | 0.01 |
| Furathiocarb | 20 | 20 | 20 | 0.01 |
| Furmecyclox | 17 | 20 | 20 | 0.05 |
| Griseofulvin | 20 | 20 | 20 | 0.01 |
| Halofenozide | 0 | 0 | 19 | 0.2 |
| Haloxyfop-2-ethoxyethyl | 20 | 20 | 20 | 0.01 |
| Haloxyfop-methyl | 20 | 20 | 20 | 0.01 |
| Heptenophos | 20 | 20 | 20 | 0.01 |
| Hexazinone | 8 | 20 | 20 | 0.05 |
| Hexythiazox | 20 | 20 | 20 | 0.01 |
| Hydramethylnon | 0 | 19 | 20 | 0.05 |
| Imazalil | 20 | 20 | 20 | 0.01 |
| Imazamethabenz-methyl | 0 | 0 | 19 | 0.2 |
| Imazamox | 0 | 3 | 19 | 0.2 |
| Imazapic | 11 | 17 | 20 | 0.2 |
| Imazaquin | 19 | 20 | 20 | 0.01 |
| Imazethapyr | 12 | 20 | 20 | 0.05 |
| Imazosulfuron | 19 | 20 | 20 | 0.01 |
| Imibenconazole | 0 | 19 | 20 | 0.05 |
| Imidacloprid-guanidine | 2 | 4 | 20 | 0.2 |
| Imidacloprid-urea | 0 | 0 | 11 | > 0.2 |
| Indanofan | 0 | 0 | 16 | > 0.2 |
| Indaziflam | 20 | 20 | 20 | 0.01 |
| Iodosulfuron-methyl | 20 | 20 | 20 | 0.01 |
| Iprovalicarb | 1 | 17 | 20 | 0.2 |
| Isocarbophos | 0 | 13 | 20 | 0.2 |
| Isofenphos | 20 | 20 | 20 | 0.01 |
| Isofenphos-methyl | 0 | 9 | 20 | 0.2 |
| Isofenphos-oxon | 20 | 20 | 20 | 0.01 |
| Isomethiozin | 20 | 20 | 20 | 0.01 |
| Isonoruron | 20 | 20 | 20 | 0.01 |
| Isopropalin | 15 | 20 | 20 | 0.05 |
| Isoprothiolane | 13 | 20 | 20 | 0.05 |
| Isoproturon | 0 | 0 | 20 | 0.2 |
| Isopyrazam | 20 | 20 | 20 | 0.01 |
| Isoxaben | 4 | 20 | 20 | 0.05 |
| Isoxadifen-ethyl | 0 | 0 | 18 | > 0.2 |
| Isoxathion | 18 | 20 | 20 | 0.05 |
| Ivermectin B1a | 0 | 3 | 20 | 0.2 |
| Kadethrin | 0 | 19 | 20 | 0.05 |
| Karbutilate | 19 | 20 | 20 | 0.01 |
| Kresoxim-methyl | 0 | 0 | 18 | > 0.2 |
| Lactofen | 20 | 20 | 20 | 0.01 |
| Leptophos | 0 | 0 | 20 | 0.2 |
| Linuron | 20 | 20 | 20 | 0.01 |
| Malaoxon | 20 | 20 | 20 | 0.01 |
| Malathion | 0 | 0 | 20 | 0.2 |
| Mandipropamid | 20 | 20 | 20 | 0.01 |
| Mefenpyr-diethyl | 20 | 20 | 20 | 0.01 |
| Mepanipyrim | 20 | 20 | 20 | 0.01 |
| Mephospholan | 20 | 20 | 20 | 0.01 |
| Mepronil | 20 | 20 | 20 | 0.01 |
| Mesosulfuron-methyl | 20 | 20 | 20 | 0.01 |
| Metaflumizone | 18 | 20 | 20 | 0.05 |
| Metalaxyl | 20 | 20 | 20 | 0.01 |
| Metamitron | 0 | 0 | 11 | > 0.2 |
| Metazachlor | 0 | 16 | 20 | 0.2 |
| Metconazole | 20 | 20 | 20 | 0.01 |
| Methabenzthiazuron | 20 | 20 | 20 | 0.01 |
| Methidathion | 0 | 0 | 20 | 0.2 |
| Methoprene | 0 | 0 | 0 | undetectable |
| Methoprotryne | 20 | 20 | 20 | 0.01 |
| Methoxyfenozide | 0 | 0 | 13 | > 0.2 |
| Metobromuron | 20 | 20 | 20 | 0.01 |
| Metosulam | 20 | 20 | 20 | 0.01 |
| Metoxuron | 0 | 18 | 20 | 0.2 |
| Metrafenone | 20 | 20 | 20 | 0.01 |
| Metribuzin | 2 | 20 | 20 | 0.05 |
| Metsulfuron-methyl | 20 | 20 | 20 | 0.01 |
| Monalide | 20 | 20 | 20 | 0.01 |
| Monolinuron | 6 | 20 | 20 | 0.05 |
| Monuron | 16 | 20 | 20 | 0.05 |
| Moxidectin | 0 | 0 | 13 | > 0.2 |
| Myclobutanil | 0 | 5 | 12 | > 0.2 |
| Napropamide | 20 | 20 | 20 | 0.01 |
| N-desethyl-pirimiphos-methyl | 20 | 20 | 20 | 0.01 |
| Neburon | 16 | 20 | 20 | 0.05 |
| Nitenpyram | 13 | 19 | 20 | 0.05 |
| Nitralin | 5 | 20 | 20 | 0.05 |
| Norflurazon | 20 | 20 | 20 | 0.01 |
| Nuarimol | 10 | 20 | 20 | 0.05 |
| O,S-TEPP | 20 | 20 | 20 | 0.01 |
| Octhilinone | 18 | 20 | 20 | 0.05 |
| Ofurace | 20 | 20 | 20 | 0.01 |
| Orbencarb | 20 | 20 | 20 | 0.01 |
| Oryzalin | 0 | 20 | 20 | 0.05 |
| Oxasulfuron | 9 | 20 | 20 | 0.05 |
| Oxaziclomefone | 20 | 20 | 20 | 0.01 |
| Paclobutrazol | 20 | 20 | 20 | 0.01 |
| Paraoxon-ethyl | 20 | 20 | 20 | 0.01 |
| Paraoxon-methyl | 0 | 20 | 20 | 0.05 |
| Penconazole | 20 | 20 | 20 | 0.01 |
| Pencycuron | 20 | 20 | 20 | 0.01 |
| Penflufen | 15 | 20 | 20 | 0.05 |
| Penoxsulam | 20 | 20 | 20 | 0.01 |
| Pentanochlor | 16 | 18 | 17 | > 0.2 |
| Penthiopyrad | 20 | 20 | 20 | 0.01 |
| Pethoxamid | 20 | 20 | 20 | 0.01 |
| Permethrin,cis | 0 | 0 | 0 | undetectable |
| Permethrin,trans | 0 | 0 | 0 | undetectable |
| Phorate-sulfone | 0 | 0 | 20 | 0.2 |
| Phosfolan | 20 | 20 | 20 | 0.01 |
| Phosfolan-methyl | 20 | 20 | 20 | 0.01 |
| Phosphamidon | 20 | 20 | 20 | 0.01 |
| Phthalicacid,benzylbutylester | 0 | 20 | 20 | 0.05 |
| Picolinafen | 20 | 20 | 20 | 0.01 |
| Picoxystrobin | 0 | 0 | 20 | 0.2 |
| Piperalin | 20 | 20 | 20 | 0.01 |
| Piperonyl butoxide | 2 | 20 | 20 | 0.05 |
| Piperophos | 20 | 20 | 20 | 0.01 |
| Pirimicarb | 20 | 20 | 20 | 0.01 |
| Pirimiphos-ethyl | 20 | 20 | 20 | 0.01 |
| Pirimiphos-methyl | 20 | 20 | 20 | 0.01 |
| Pretilachlor | 20 | 20 | 20 | 0.01 |
| Primisulfuron-methyl | 0 | 20 | 20 | 0.05 |
| Probenazole | 8 | 20 | 20 | 0.05 |
| Prochloraz | 18 | 20 | 20 | 0.05 |
| Prodiamine | 0 | 5 | 19 | 0.2 |
| Profenofos | 20 | 20 | 20 | 0.01 |
| Profoxydim | 20 | 20 | 20 | 0.01 |
| Prometon | 20 | 20 | 20 | 0.01 |
| Prometryn | 20 | 20 | 20 | 0.01 |
| Propachlor | 20 | 20 | 20 | 0.01 |
| Propamocarb | 0 | 19 | 20 | 0.05 |
| Propanil | 0 | 20 | 20 | 0.05 |
| Propaphos | 18 | 20 | 20 | 0.05 |
| Propaquizafop | 20 | 20 | 20 | 0.01 |
| Propargite | 0 | 0 | 12 | > 0.2 |
| Propazine | 20 | 20 | 20 | 0.01 |
| Propiconazole | 20 | 20 | 20 | 0.01 |
| Propoxycarbazone | 0 | 0 | 0 | undetectable |
| Propyzamide | 0 | 20 | 19 | 0.05 |
| Proquinazid | 20 | 20 | 20 | 0.01 |
| Prosulfocarb | 0 | 17 | 19 | 0.2 |
| Prosulfuron | 20 | 20 | 20 | 0.01 |
| Prothiophos | 0 | 6 | 20 | 0.2 |
| Pymetrozine | 0 | 20 | 20 | 0.05 |
| Pyracarbolid | 20 | 20 | 20 | 0.01 |
| Pyraclofos | 20 | 20 | 20 | 0.01 |
| Pyraclostrobin | 20 | 20 | 20 | 0.01 |
| Pyraflufen-ethyl | 20 | 20 | 20 | 0.01 |
| Pyrasulfotole | 0 | 0 | 18 | > 0.2 |
| Pyrazophos | 20 | 20 | 20 | 0.01 |
| Pyrazosulfuron-ethyl | 20 | 20 | 20 | 0.01 |
| Pyrazoxyfen | 20 | 20 | 20 | 0.01 |
| Pyributicarb | 20 | 20 | 20 | 0.01 |
| Pyridaben | 14 | 20 | 20 | 0.05 |
| Pyridalyl | 17 | 20 | 20 | 0.05 |
| Pyridaphenthion | 20 | 20 | 20 | 0.01 |
| Pyrifenox-1 | 20 | 20 | 20 | 0.01 |
| Pyrifenox-2 | 20 | 20 | 20 | 0.01 |
| Pyriftalid | 20 | 20 | 20 | 0.01 |
| Pyrimethanil | 20 | 20 | 20 | 0.01 |
| Pyriproxyfen | 20 | 20 | 20 | 0.01 |
| Pyrithiobac | 0 | 17 | 20 | 0.2 |
| Pyroquilon | 20 | 20 | 20 | 0.01 |
| Pyroxasulfone | 20 | 20 | 20 | 0.01 |
| Pyroxsulam | 20 | 20 | 20 | 0.01 |
| Quinalphos | 0 | 13 | 19 | 0.2 |
| Quinoclamine | 0 | 20 | 20 | 0.05 |
| Quinoxyfen | 20 | 20 | 20 | 0.01 |
| Quizalofop-ethyl | 20 | 20 | 20 | 0.01 |
| Rabenzazole | 20 | 20 | 20 | 0.01 |
| Resmethrin | 2 | 18 | 20 | 0.2 |
| Rimsulfuron | 0 | 4 | 20 | 0.2 |
| Rotenone | 20 | 20 | 20 | 0.01 |
| Saflufenacil | 17 | 20 | 20 | 0.05 |
| Sebuthylazine | 20 | 20 | 20 | 0.01 |
| Sebuthylazine-desethyl | 13 | 18 | 20 | 0.2 |
| Secbumeton | 0 | 0 | 0 | undetectable |
| Sethoxydim | 11 | 20 | 20 | 0.05 |
| Siduron | 0 | 20 | 20 | 0.05 |
| Silthiofam | 20 | 20 | 20 | 0.01 |
| Simazine | 20 | 20 | 20 | 0.01 |
| Simeconazole | 20 | 20 | 20 | 0.01 |
| Simeton | 20 | 20 | 20 | 0.01 |
| Simetryn | 20 | 20 | 20 | 0.01 |
| S-Metolachlor | 20 | 20 | 20 | 0.01 |
| Spinetoram | 0 | 20 | 20 | 0.05 |
| Spinosad A/D | 3 | 15 | 20 | 0.2 |
| Spirokamine | 20 | 20 | 20 | 0.01 |
| Spiromesifen | 0 | 1 | 19 | 0.2 |
| Spirotetramat | 20 | 20 | 20 | 0.01 |
| Spiroxamine | 20 | 20 | 20 | 0.01 |
| Sulcotrione | 0 | 0 | 18 | > 0.2 |
| Sulfentrazone | 0 | 0 | 0 | undetectable |
| Sulfometuron-methyl | 17 | 18 | 20 | 0.2 |
| Sulfosulfuron | 18 | 20 | 20 | 0.05 |
| Sulfotep | 20 | 20 | 20 | 0.01 |
| Sulprofos | 20 | 20 | 20 | 0.01 |
| TCMTB | 17 | 20 | 20 | 0.05 |
| Tebuconazole | 20 | 20 | 20 | 0.01 |
| Tebufenpyrad | 20 | 20 | 20 | 0.01 |
| Tebupirimfos | 20 | 20 | 20 | 0.01 |
| Tebutam | 20 | 20 | 20 | 0.01 |
| Tebuthiuron | 1 | 20 | 20 | 0.05 |
| Tefluthrin | 20 | 19 | 20 | 0.01 |
| Temephos | 20 | 20 | 20 | 0.01 |
| Tepraloxydim | 19 | 20 | 20 | 0.01 |
| Terbufos-sulfone | 0 | 0 | 17 | > 0.2 |
| Terbufos-sulfoxide | 0 | 20 | 20 | 0.05 |
| Terbumeton | 20 | 20 | 20 | 0.01 |
| Terbuthylazine-desethyl | 0 | 11 | 19 | 0.2 |
| Terbutryn | 20 | 20 | 20 | 0.01 |
| Tetraconazole | 20 | 20 | 20 | 0.01 |
| Tetramethrin | 0 | 20 | 20 | 0.05 |
| Thenylchlor | 0 | 0 | 14 | > 0.2 |
| Thiabendazole | 14 | 20 | 20 | 0.05 |
| Thiabendazole-5-hydroxy | 3 | 20 | 20 | 0.05 |
| Thiacloprid | 6 | 20 | 20 | 0.05 |
| Thiamethoxam | 9 | 20 | 20 | 0.05 |
| Thiazopyr | 20 | 20 | 20 | 0.01 |
| Thidiazuron | 0 | 18 | 20 | 0.2 |
| Thiencarbazone-methyl | 0 | 0 | 0 | undetectable |
| Thifensulfuron-methyl | 20 | 20 | 20 | 0.01 |
| Thiodicarb | 20 | 20 | 20 | 0.01 |
| Thiophanate-ethyl | 19 | 20 | 20 | 0.01 |
| Thiophanate-methyl | 19 | 20 | 20 | 0.01 |
| Tolclofos-methyl | 0 | 20 | 20 | 0.05 |
| Tolfenpyrad | 18 | 20 | 20 | 0.05 |
| Tralkoxydim | 16 | 20 | 20 | 0.05 |
| Triadimefon | 17 | 20 | 20 | 0.05 |
| Tri-allate | 0 | 19 | 20 | 0.05 |
| Triasulfuron | 19 | 20 | 20 | 0.01 |
| Triazophos | 0 | 0 | 0 | undetectable |
| Triazoxide | 20 | 20 | 20 | 0.01 |
| Tribufos (DEF) | 20 | 20 | 20 | 0.01 |
| Trichlorfon | 0 | 19 | 20 | 0.05 |
| Tricyclazole | 17 | 20 | 20 | 0.05 |
| Tridemorph | 14 | 18 | 20 | 0.2 |
| Trietazine | 20 | 20 | 20 | 0.01 |
| Trifloxystrobin | 20 | 20 | 20 | 0.01 |
| Trifloxysulfuron | 20 | 20 | 20 | 0.01 |
| Triflumizole | 0 | 20 | 20 | 0.05 |
| Triflumuron | 20 | 20 | 20 | 0.01 |
| Triflusulfuron-methyl | 20 | 20 | 20 | 0.01 |
| Tritosulfuron | 11 | 20 | 20 | 0.05 |
| Valifenalate-1 | 11 | 20 | 20 | 0.05 |
| Valifenalate-2 | 14 | 20 | 20 | 0.05 |
| Vernolate | 0 | 20 | 20 | 0.05 |
| Zoxamide | 20 | 20 | 20 | 0.01 |



**Figure S1** Labile paraoxon-ethyl as an example for illustrating effects of the reduced capillary voltage, sampling cone voltage and low-energy channel voltage on fragmentations in the full scan.

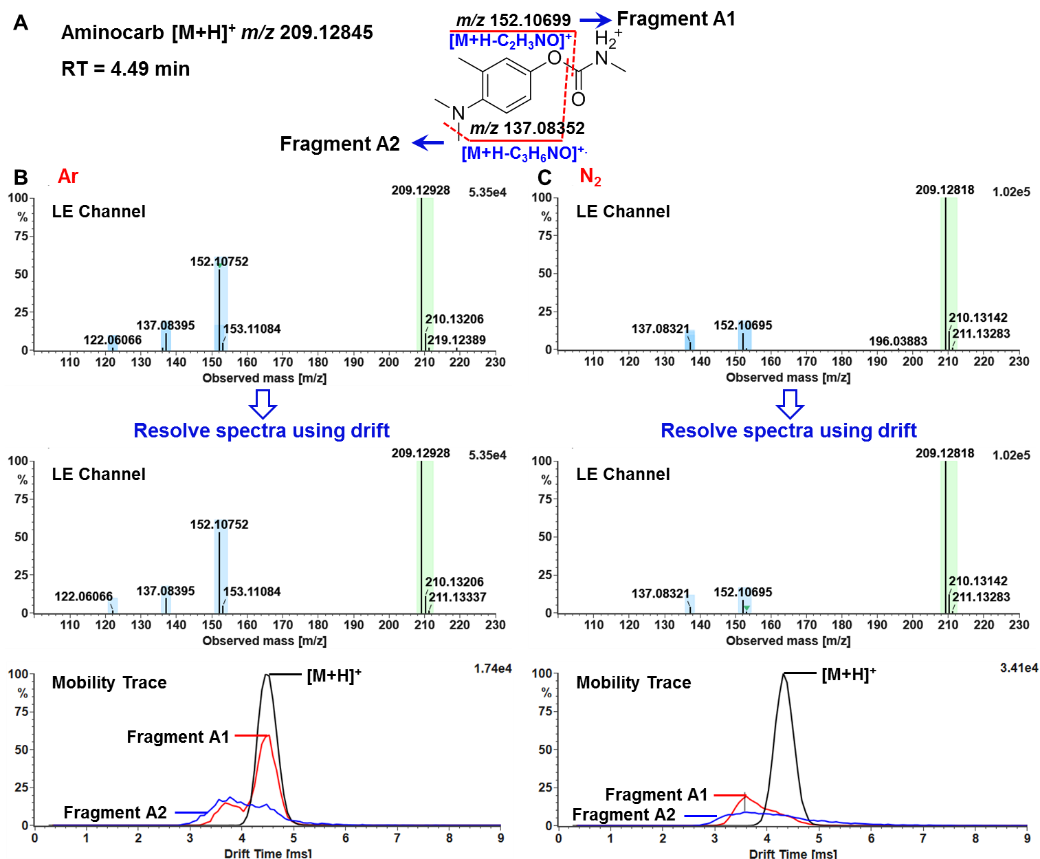
(A: the proposed fragmentation pathway of paraoxon-ethyl; B: comparison of the low-energy channel spectra with the capillary voltage settings of 0.5 eV and 2.5 eV; C: comparison of the low-energy channel spectra with the sampling cone voltage settings of 10 V and 40 V; D: comparison of the low-energy channel spectra with the low-energy channel voltage settings of 4 eV and 6 eV)



**Figure S2** Labile paraoxon-ethyl as an example for illustrating effects of collision gas on fragmentations in the full scan.

(The proposed fragmentation of paraoxon-ethyl to produce Fragment P1 (*m/z* 220.00055) and Fragment P2 (*m/z* 248.03185) (A); the low-energy (LE) spectra of *m/z* 276.06315 with argon (B) and nitrogen (C) as collision gas, respectively.)

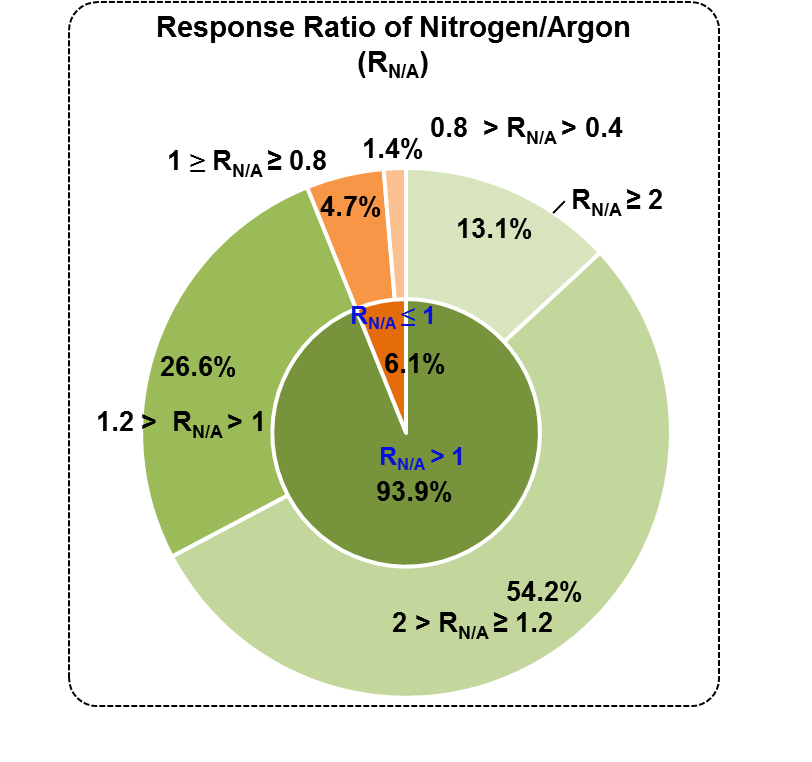
The labile paraoxon-ethyl was easy to fragment into two intense ions of *m/z* 220.00055 (Fragment P1) and 248.03185 (Fragment P2), of which the proposed fragmentation pathway was depicted as Figure S2.A. From the low-energy spectra, there was an obvious decrease on dissociation of the protonated ion at *m/z* 276.06315 with nitrogen as the collision gas instead of argon (Figure S2.B and Figure S2.C). In particular, the abundant Fragment P1 was absent by resolving the spectra using drift when nitrogen was applied. It suggested that the Fragment P1 and Fragment P2 filtered out were not produced in the collision cell and that the post-mobility fragmentations of the protonated ion at *m/z* 276.06315 was obviously reduced with nitrogen compared to argon.



**Figure S3** Labile aminocarb as an example for illustrating effects of collision gas on fragmentations in the full scan.

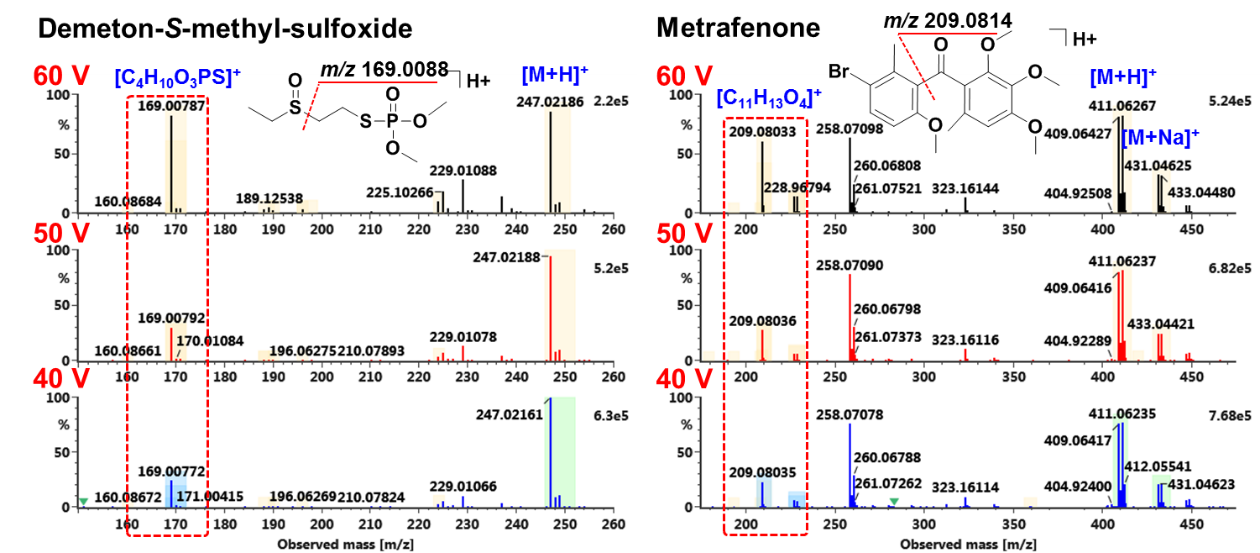
(The proposed fragmentation of aminocarb to produce Fragment A1 (*m/z* 152.10699) and Fragment A2 (*m/z* 137.08352) (A); the low-energy (LE) spectra of *m/z* 209.12845 and the overlapped mobiligram of the extracted ions of *m/z* 209.12845, 152.10699 and 137.08352 with argon (B) and nitrogen (C) as collision gas, respectively.)

With argon as the collision gas, the protonated ion of aminocarb at *m/z* 209.12845 was visibly dissociated into Fragment A1 (*m/z* 152.10699) and Fragment A2 (*m/z* 137.08352) in the low-energy (LE) spectra. And the possible fragmentation pathway was proposed in Figure S3.A. When argon was replaced with nitrogen, the abundance of Fragment A1 and Fragment A2 in the low-energy (LE) spectra obviously reduced. Comparisons of the drift time-aligned low-energy spectra and the overlapped mobiligram in the two cases evidenced that nitrogen as the collision gas significantly improved unwanted fragmentations occurred in the collision cell.

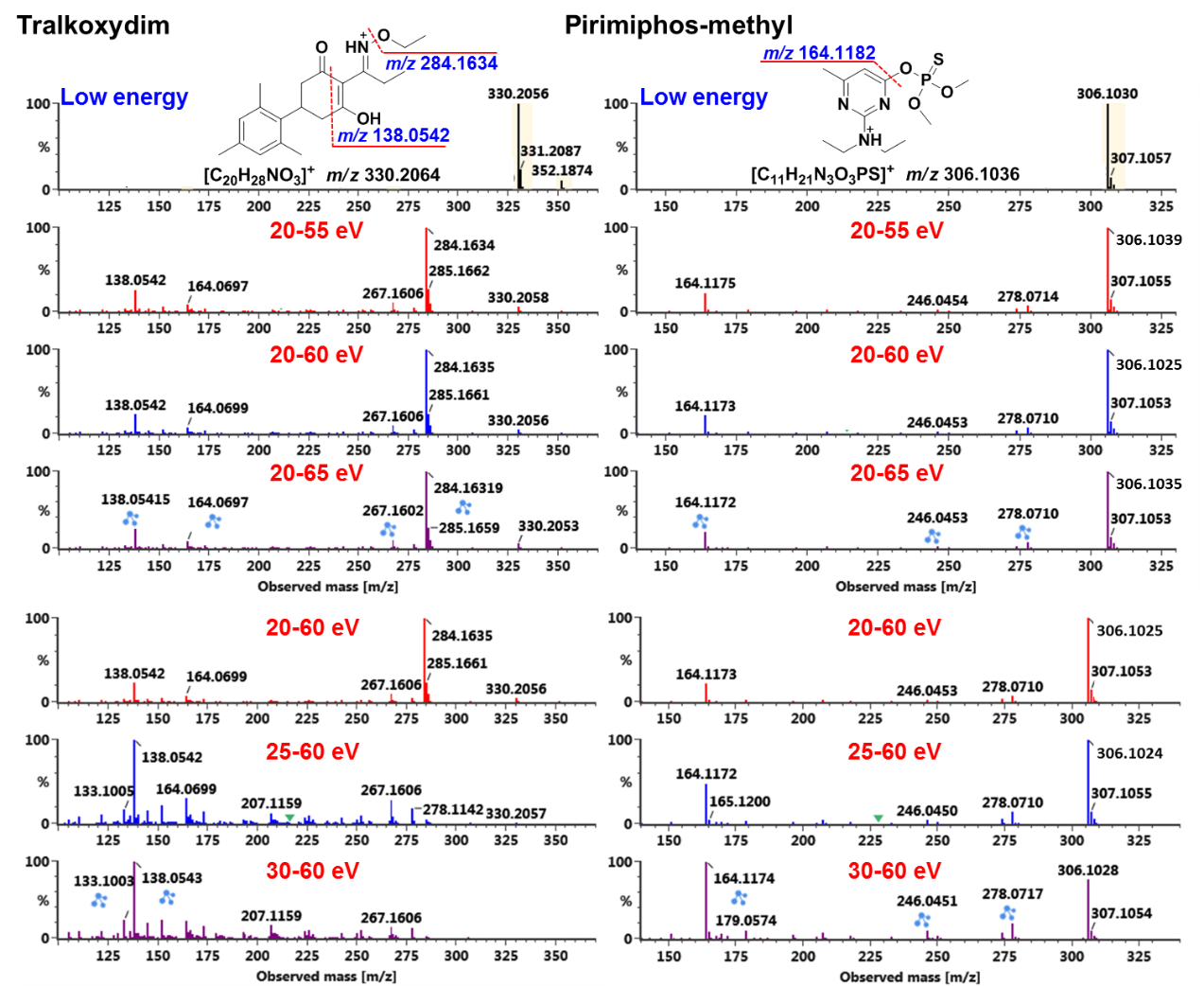


**Figure S4** Response ratio of 443 molecular ions detected with nitrogen as the collision gas to argon (RN/A)

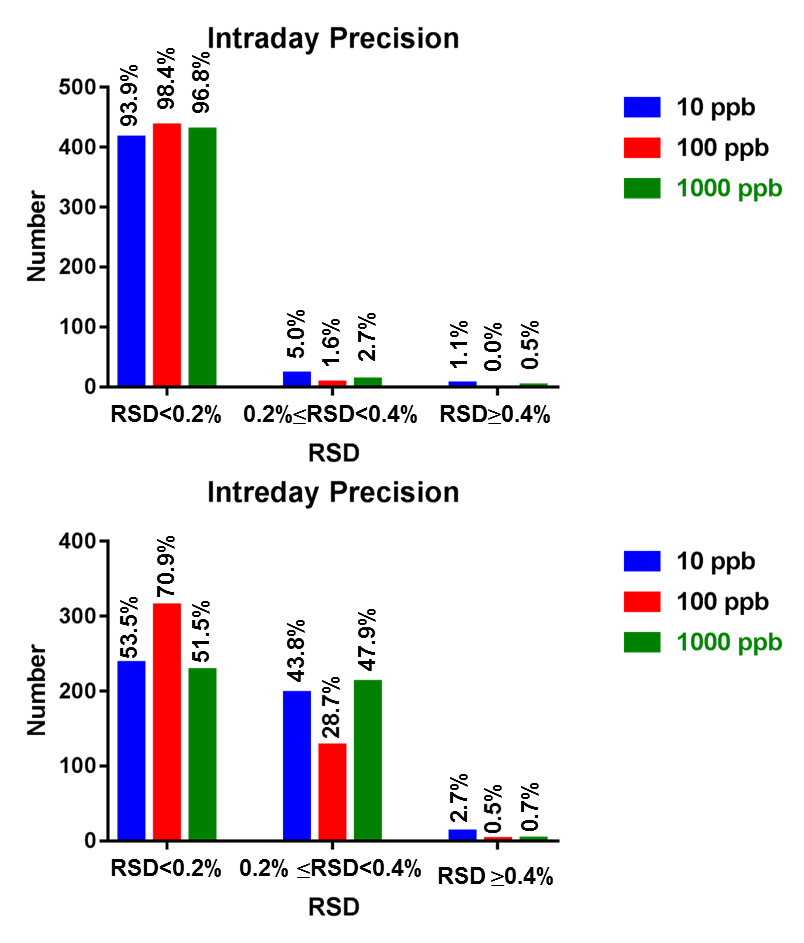
**Figure S5** The response variations of eight representative pesticides from different sub-structure types at different capillary voltage settings (0.5, 1.0, 1.5, 2.0, 2.5, 3.0 and 3.5 kV)



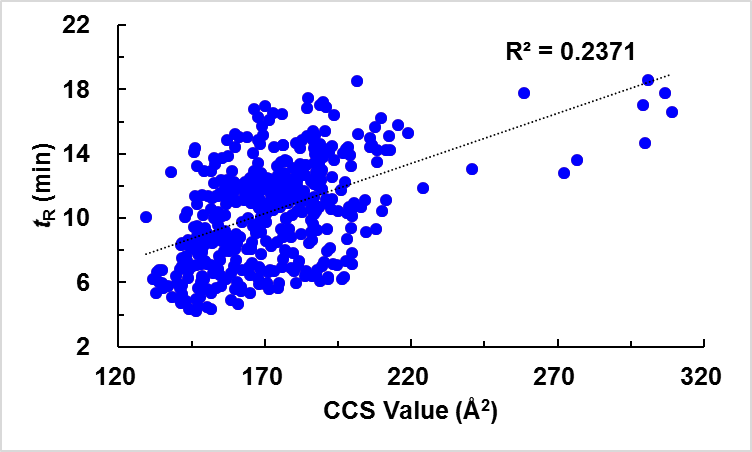
**Figure S6** The low-energy spectra of demeton-*S*-methyl-sulfoxide and metrafenone at different sampling cone voltage settings (40, 50 and 60 V)



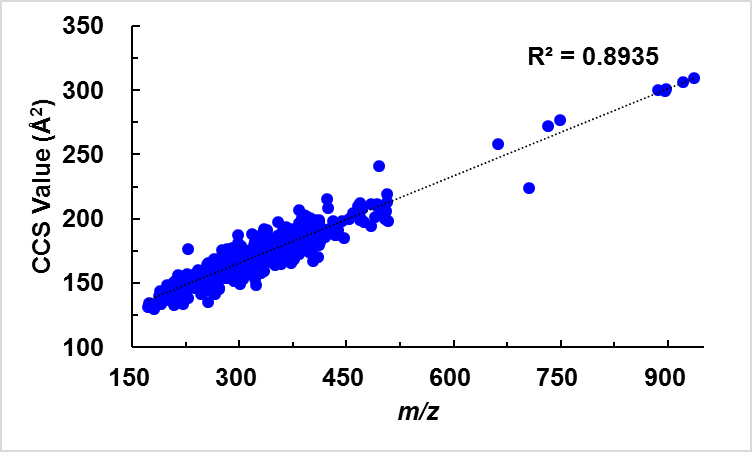
**Figure S7** The high-energy spectra of tralkoxydim and pirimiphos-methyl at different LME (20, 25 and 30 eV) and HME settings (55, 60 and 65 eV)



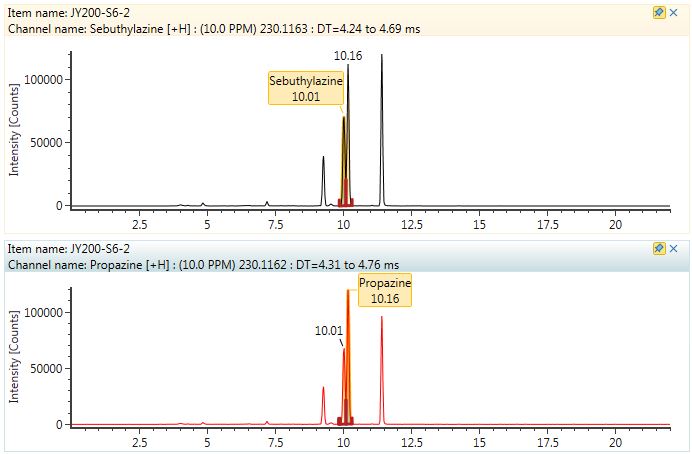
**Figure S8** The intraday precision (n=6) and interday precision (n=15) of CCS measurements



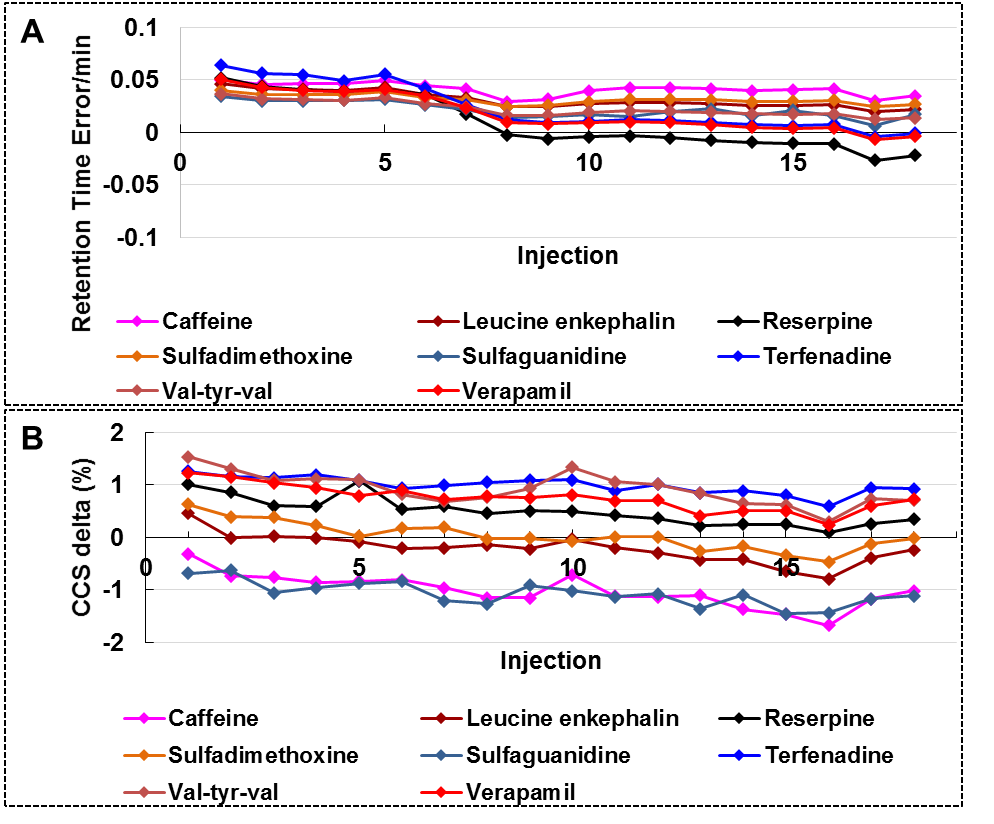
**Figure S9** A two-dimension distribution of CCS values against retention times for 443 pesticide entries (R2: linearity regression correlation coefficient)



**Figure S10** A two-dimension distribution of CCS values against *m/z* for 443 pesticide entries (R2: linearity regression correlation coefficient)



**Figure S11** The extracted ion chromatograms of sebuthylazine and propazine



**Figure S12** The retention time derivations (A) and the CCS derivations (B) of the eight compounds from the QC