**Supporting Information**

**Table S1.** Setpoints and parameters used for the Find by Fragments Algorithm

|  |  |  |  |
| --- | --- | --- | --- |
| **Section/subsection** | **Parameter** | **Action/Choice** | **Setpoint** |
| Find by Fragments/Target Source | Target Source | Choose path to desired PCDL |  |
|  | Values to match | Require RT match… | Check box |
|  | Matches per formula |  | 1 |
| Find by Fragments/Fragment Options | Fragment ion source | Use spectral library only | Highlight radio button |
|  | Fragment ion source | No. of most specific ions… | 6 |
|  | Fragment ion EIC qual settings | RT difference | 0.1 |
|  | Fragment ion EIC qual settings | S/N ratio >= | Leave box unchecked |
|  | Fragment ion EIC qual settings | Coelution score >= | 70 |
|  | Fragment ion Confirmation criteria | Minimum # qualified fragments | 2 or 1 |
| Find by Fragments/Match Tolerance | Match tolerance | Masses +/- | 5.00 mDa |
|  | Match tolerance | Retention times +/- | 0.15 min |
|  | Expansion of values for chromatogram extraction | Possible m/z | Symmetric ppm +/- 35.0 |
|  | Expansion of values for chromatogram extraction | Limit EIC extraction range | Symmetric +/- 0.40 min |
| Find by Fragments/EIC Integration | Integrator selection | Agile 2 |  |
| Find by Fragments/EIC Peak Filters | Filter on | *Check* Peak Height radio button |  |
|  | Height filters | Absolute height >= | 100 |
|  | Height filters | Relative height >= | Unchecked |
|  | Maximum number of peaks | Limit by height to the largest | 100 |
| Find by Fragments/Fragment Peak Filter | Height filters | *Check* Absolute height >= | 30 counts |
|  | Maximum number of peaks | *Check* Limit (by height) to the largest | 100 |
| Find by Fragments/Results | Previous results | Clear previous results | Check box |
|  | New results | *Check* either radio button |  |
|  | Extract results | Extract complete result set automatically | Check box |
| Identification/Generate Formulas | Allowed Species | Positive ions | *Check* -electron; uncheck others |
|  | Allowed Species | Elements and limits | Add any elements that could be found in a target compound formula |
|  | Charge state | Limit assigned charge state to a range of | *Check* box and enter 1 |
| Method Automation/Workflow | Options | Choose Target/Suspect Screening |  |
|  | Compound mining | Choose Find by Fragments |  |
|  | Target Source | Choose path to desired PCDL |  |
|  |  | Require RT match if database contains RT for target compound | Check box |
|  |  | Only report qualified compounds | Check box |

**Table S2.** Average number of Qualified Compounds found by the Find by Fragments (FbF) algorithm and Unknowns Analysis using the complete 1020-compound PCDL or the 250-compound subset PCDL when analyzing 21 samples of confiscated cannabis. When using FbF, the minimum number of qualified fragments was set to 2.

|  |  |  |
| --- | --- | --- |
|  | Using the P&EP 1020- compound PCDL | Using the 250-compound subset PCDL |
| Find by Fragments Extraction of 6 Ions Using a Minimum Coelution Score of 70. Minimum number of qualified fragments = 2 | 71 | 15 |
| Unknowns Analysis | 15 | 3 |

**Table S3.** Pesticides spiked into a solvent-diluted cannabis extract at 9 different levels. Showing the number of qualified ions (6 were extracted) for each pesticide at each concentration, detection levels in the diluted samples and the equivalent concentration in a cannabis sample (assuming 100% recovery) and California’s required detection limits. California residue tolerances highlighted in yellow are for compounds that could be found at the tolerance level using this method by identifying at least two characteristic ions for the pesticide residue.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Pesticides Spiked into Diluted (125:1) Cannabis Extract** | | **Concentration of Pesticides Spiked into an Organically-Grown-Cannabis Extract** | | | | | | | | | | | | |  | | **Summary** | | |  |
| Compound | Retention time (min) | 50 ppb | 25 ppb | 10 ppb | 5 ppb | 2.5 ppb | 1 ppb | | | 0.8 ppb | | 0.5 ppb | 0.3 ppb | | Lowest Detection Level in diluted extract (ppb) | | Lowest Detection Level in Cannabis (ppb)a | | California residue Tolerances (ppb)b, c | |
| Acephate | 5.658 | 6e | 6 | 6 | 6 | 5 | 2+ | | | 3 | | 3 |  | | 0.5 | | 62.5 | | 100/3000 | |
| Azoxystrobin | 18.408 | 5 | 2 |  |  |  |  | | |  | |  |  | | 25 | | 3125 | | 100/400000 | |
| Bifenthrin | 13.913 | 6 | 6 | 4+ | 3 | 6 | 6 | | | 3 | | 6 | 6 | | 0.3 | | 37.5 | | 3000/500 | |
| Boscalid | 16.580 | 4 | 3 | 3 | 2+ | 3 | 3 | | | 3 | | 3 |  | | 0.5 | | 62.5 | | 100/10000 | |
| Captan | 10.726 | 5 | 4 | 2+ | 2+ |  |  | | |  | |  |  | | 5 | | 625 | | 7000/5000 | |
| Carbaryl | 9.231 | 6 | 6 | 5 | 4 | 2+ | 3 | | | 3 | | 4 | 3 | | 0.3 | | 37.5 | | 500/500 | |
| Carbofuran | 7.843 | 4 | 4 | 2+ | 3+ | 5 | 5 | | | 4 | | 5 | 4 | | 0.3 | | 37.5 | | 100 | |
| Chlordane-trans  Chlordane-cis | 11.033  11.291 | 6 | 5 | 3+ | 4+ |  |  | | | 2+ | |  |  | | 5 | | 625 | | 100 | |
| Chlorfenapyr | 12.036 | 6 | 5 | 4+ | 3 | 3 | 2+ | | |  | |  |  | | 1 | | 125 | | 100 | |
| Chlorpyrifos | 9.954 | 6 | 6 | 6 | 6 | 6 | 6 | | | 6 | | 3+ | 5 | | 0.3 | | 37.5 | | 100 | |
| Coumaphos | 15.853 | 6 | 5 | 2+ | 3 |  |  | | |  | |  |  | | 5 | | 625 | | 100 | |
| Cyfluthrin | 16.172, 16.253, 16.343, 16.367 | 5 | 2 | 2 | 3 | 2 | 3 | | | 2 | | 3 | 2 | | 0.3 | | 37.5 | | 2000/1000 | |
| Cypermethrind | 16.483, 16.569, 16.649, 16.680 | 3 |  |  |  |  |  | | |  | |  |  | | 50 | | 6250 | | 1000/1000 | |
| Diazinon | 8.285 | 6 | 6 | 6 | 6 | 6 | 5+ | | | 5 | | 5 | 4 | | 0.3 | | 37.5 | | 100/200 | |
| Dichlorvos | 4.679 | 6 | 6 | 6 | 6 | 6 | 6 | | | 6 | | 6 | 6 | | 0.3 | | 37.5 | | 100 | |
| Dimethoate | 7.791 | 6 | 5 | 5 | 5 | 4 | 4+ | | | 4 | | 4 | 4 | | 0.3 | | 37.5 | | 100 | |
| Dimethomorph | 18.457, 18.702 | 4+ | 3+ | 2 | 2 |  |  | | |  | |  |  | | 5 | | 625 | | 2000/20000 | |
| Ethoprop | 7.021 | 6 | 6 | 6 | 6 | 6 | 6 | | | 6 | | 5 | 5 | | 0.3 | | 37.5 | | 100 | |
| Etofenprox | 16.777 | 4 | 4 | 3 | 3 | 3 | 2 | | | 2 | | 3 | 3 | | 0.3 | | 37.5 | | 100 | |
| Fenhexamid | 13.032 | 6 | 6 | 2+ |  |  |  | | |  | |  |  | | 10 | | 1250 | | 100/10000 | |
| Fipronil | 10.639 | 6 | 6 | 6 | 5 | 4+ | 3+ | | | 3+ | | 3 | 2+ | | 0.3 | | 37.5 | | 100 | |
| Flonicamid | 6.698 | 6 | 6 | 6 | 5 | 5 | 5 | | | 5 | | 4 | 3 | | 0.3 | | 37.5 | | 100/2000 | |
| Fludioxonil | 11.527 | 6 | 6 | 6 | 6 | 6 | 4 | | | 3 | | 3 |  | | 0.5 | | 62.5 | | 100/30000 | |
| Imazalil | 11.480 | 6 | 5 | 4+ | 4 |  |  | | |  | |  |  | | 5 | | 625 | | 100 | |
| Kinoprene | 9.729 | 5 | 4 | 5 | 5 | 5 | 5 | | | 5 | | 5 | 5 | | 0.3 | | 37.5 | | f | |
| Kresoxim-methyl | 11.806 | 6 | 6 | 4 | 4 | 4 | 4 | | | 3 | | 4 | 2 | | 0.3 | | 37.5 | | 100/1000 | |
| Malathion | 9.729 | 6 | 6 | 5 | 6 | 5 | 5 | | | 4 | | 4 | 4 | | 0.3 | | 37.5 | | 500/5000 | |
| Metalaxyl | 9.328 | 6 | 6 | 6 | 6 | 6 | 2+ | | |  | |  |  | | 1 | | 125 | | 2000/15000 | |
| Methiocarb | 9.576 | 5 | 5 | 5 | 5 | 4 | 2+ | | | 2+ | | 2+ | 2 | | 0.3 | | 37.5 | | 100 | |
| Methyl parathion | 9.139 | 6 | 6 | 6 | 6 | 5 | 5 | | | 3+ | | 3+ | 2+ | | 0.3 | | 37.5 | | 100 | |
| Mevinphos | 5.610 | 6 | 6 | 6 | 6 | 6 | 5 | | | 6 | | 4+ | 4 | | 0.3 | | 37.5 | | 100 | |
| MGK-264 | 10.432 | 6 | 6 | 6 | 5 | 3+ | 2+ | | | 2+ | | 3 |  | | 0.5 | | 62.5 | | f | |
| Myclobutanil | 11.718 | 6 | 6 | 6 | 6 | 2+ |  | | |  | |  |  | | 2.5 | | 312.5 | | 100/9000 | |
| Naled | 7.248 | 6 | 6 | 5 | 5 | 3 |  | | |  | |  |  | | 2.5 | | 312.5 | | 100/500 | |
| Pentachloro-nitrobenzene | 8.235 | 6 | 6 | 6 | 6 | 6 | 5 | | | 6 | | 6 | 2+ | | 0.3 | | 37.5 | | 100/200 | |
| Permethrin | 15.602, 15.726 | 6 | 3+ | 4 | 4 | 3 | 4 | | | 3 | | 4 | 3 | | 0.3 | | 37.5 | | 500/20000 | |
| Phosmet | 13.899 | 4 | 4 | 4 |  |  |  | | |  | |  |  | | 10 | | 1250 | | 100/200 | |
| Piperonyl butoxide | 13.364 | 4 | 3 |  |  | 2 |  | | |  | |  |  | | 20 | | 2500 | | 3000/8000 | |
| Propiconazole | 12.927, 13.042 | 6 | 6 | 6 | 6 | 3+ |  | | |  | |  |  | | 2.5 | | 312.5 | | 100/20000 | |
| Propoxur | 6.843 | 5 | 5 | 5 | 3 | 3 | 2 | | | 2 | | 3 | 2 | | 0.3 | | 37.5 | | 100 | |
| Pyridaben | 15.768 | 4 | 4 | 2+ | 2+ |  |  | | |  | |  |  | | 5 | | 625 | | 100/3000 | |
| Spiroxamine | 9.077, 9.535 | 6 | 5 | 5 | 5 | 4 | 2+ | | | 2+ | | 4 |  | | 0.5 | | 62.5 | | 100 | |
| Tebuconazol | 13.266 | 6 | 6 | 6 | 5 | 3 | 2 | | |  | |  |  | | 1 | | 125 | | 100/2000 | |
| Thiamethoxam | 10.275 | 6 | 6 | 4+ | 2+ |  |  | | |  | |  |  | | 5 | | 625 | | 5000/4500 | |
| Trifloxystrobin | 12.940 | 4 | 4 | 2 | 2 | 2 |  | | |  | |  |  | | 2.5 | | 312.5 | | 100/30000 | |
| **45 total pesticides** |  | **45 found** | **44 found** | **43 found** | **40 found** | **33 found** | **30 found** | | | **28 found** | | **26 found** | **21 found** | |  | |  | |  | |
| a) Lowest detectable concentration multiplied by 125 to correct for the dilution factor | | | | | | | | | | |  |  | |  |  |  | |  | | | |  |  |  |  |  |  |  |  |  |  |
| b) BUREAU OF CANNABIS CONTROL TEXT OF REGULATIONS, CALIFORNIA CODE OF REGULATIONS, TITLE 16, DIVISION 42. BUREAU OF CANNABIS CONTROL; <https://www.bcc.ca.gov/law_regs/readopt_text_final.pdf> | | | | | | | | | | | | | | | | | | | | | |  |  |  |  |  |  |  |  |  |  |
| c) Values of 100 ppb are given for California Category I Pesticides. Values X/Y are for Category II Pesticides where X is for inhalable cannabis goods and Y is for other cannabis goods. | | | | | | | |  |  | |  |  | |  |  |  | |  | | | |  |  |  |  |  |  |  |  |  |  |
| d) Cypermethrin has four diastereomers so the nominal concentration of each isomer is about 1/4 of the values shown in row 2. | | | | | | | | | | | | | | | | | | | | | | | |  |  |  |  |  |  |  |  |
| e) Values shown in columns 3-11 indicate the number of ions detected by the Find by Fragments algorithm. Values shown with a + (e.g., 2+, 3+) indicate that one or more peaks were discernable in the EICs above the noise, but they were not integrated. | | | | | | | | | | | | | | | |  | |  | | | |  |  |  |  |  |  |  |  |  |  |
| f) California does not have a maximum residue limit for this compound. | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |