

Pesticide residues screening and quantitation analysis in olive oil using an Orbitrap Exploris 240 HRMS

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Goal

To develop and test a multi-residue instrument method that can be applied for high-throughput quantitation and unknown screening of pesticide residues in food matrices at or below the current legislative requirements. A high-resolution, accurate-mass (HRAM) mass spectrometer was operated in Full Scan-Data-Independent Acquisition (DIA) mode and using a Thermo Scientific™ AcquireX™ Background Exclusion workflow, providing an option for full spectrum filtering, retrospective analysis, and multi-parameter-based compound identification. The method was tested on over 400 target pesticides, in positive and negative mode, with an option for future extension to a larger number of analytes.



Introduction

The demand for quick and simple analysis of large numbers of samples in agriculture applications is growing yearly. Throughout the world, pesticides are used to control pests that are harmful to crops, humans, and animals. These substances can pose a significant health threat, and therefore need to be accurately detected at the levels required by governmental authorities. Typically, maximum residue levels for pesticides in different products of plant and animal origin are set at low part-per-billion (ppb) levels. The current regulations present significant analytical challenges with respect to the low limits of quantification and high number of target analytes.

Most routine LC-based methods usually employ triple quadrupole mass spectrometry. In recent years, Thermo Scientific™ Orbitrap™ mass analyzers have become available, providing higher confidence in compound identification and confirmation along with quantitative capabilities comparable to triple quadrupole MS/MS. Mass accuracy (typically below 5 ppm) minimizes interferences from co-eluting analytes and matrix co-extractives, and thus reduces the potential for false positive and negative results. This work describes the method performance parameters using the latest benchtop LC-Orbitrap instrument, the Thermo Scientific™ Orbitrap Exploris™ 240 mass spectrometer and its application to screening hundreds of target analytes at or below legislative levels (maximum residue levels – MRLs) in olive oil matrix.

Experimental

Reagents, all Fisher Scientific

- Acetonitrile, uHPLC-MS grade (P/N A956-1)
- Ammonium formate >99% (P/N A115-50)
- Methanol, uHPLC-MS grade (P/N A458-1)
- Formic acid, extra pure for HPLC (P/N 28905)
- Water, uHPLC-MS grade (P/N W8-1)

Consumables

- Thermo Scientific™ HPLC Vial (P/N A4954-010)
- Thermo Scientific™ National™ 10 mm Wide Opening Screw Caps and Septa (P/N C4010-60A)
- Thermo Scientific™ Accucore™ aQ column, 100 × 2.1 mm, 2.6 μm (P/N 17326-102130)

Standards

Pesticides were purchased from Ultra Scientific. See results tables for the identity of all pesticides investigated for targeted analysis.

Sample preparation

Olive oil was purchased from a local market and analyzed for background levels of pesticides. Approximately 5 g of olive oil was weighed into a 50 mL conical tube. Then, 10 mL of acetonitrile, 6 mL of water, and 100 μL of internal standard were added to the tube. This mixture was capped and shaken vigorously for 5 minutes. A Thermo Scientific™ QuEChERS™ salt slim pack (4000 mg MgSO₄, 1000 mg NaCl, 500 mg Na₂ citrate and 1000 mg Na₃ citrate), which includes all the salts required for the extraction process, was added. The mixture was shaken for about 1 minute and then centrifuged at >3300 rpm for 15 minutes. A 2 mL aliquot of the supernatant was aspirated and filtered through a 0.45 μm filter into a vial. The recovered supernatant was passed through a lipid removal cartridge into an HPLC vial and spiked with the necessary calibration levels. A 1 μL injection was made with the Thermo Scientific™ Vanquish™ Flex Binary UHPLC system equipped with a Thermo Scientific™ Accucore™ aQ reversed phase column.

Calibration standard preparation

A MegaMix high stock standard was prepared by taking 10 μL from each vial (~1000 μg/mL) and adding them together. For calibration, a 5-level calibration set was prepared by post-spiking the control olive oil extract with the mixture at concentrations ranging from 0.5 to 500 (0.5, 1.0, 5, 10, 500) ppb. All calibration levels were injected six times.

Instrument analysis

Sample analysis was carried out on a Vanquish Flex Binary UHPLC system coupled to an Orbitrap Exploris 240 mass spectrometer.

HPLC parameters

Column temperature	30 °C
Flow rate	300 µL/min
Total run time	15 min
Injection volume	1 µL
Column	Accucore aQ, 100 × 2.1 mm, 2.6 µm
Mobile phases	A: Water with 5 mM ammonium formate, 0.1% formic acid B: Methanol with 5 mM ammonium formate, 0.1% formic acid
Gradient	Table 1

Table 1. HPLC gradient run program

Time [min]	Flow rate [mL/min]	A%	B%	Curve
0.0	0.300	98	2	5
1.0	0.300	98	2	5
2.0	0.300	50	50	5
9.0	0.300	2	98	5
12.0	0.300	2	98	5
12.1	0.300	98	2	5
15.0	0.300	98	2	5

Orbitrap Exploris 240 MS settings

Spray voltage	3.5 kV Pos / 2.5 kV Neg
Sheath gas	30 arb
Aux gas	6 arb
Sweep gas	1 arb
Capillary temperature	290 °C
Vaporizer temperature	350 °C
Ion polarity	Pos / Neg switching
Full scan mass range	110 – 1100 <i>m/z</i>
Full scan resolution	45,000
Data-Independent Acquisition (DIA) resolution	30,000
HCD collision energy	Stepped 18, 35, 60

Data acquisition and processing

Data were acquired and processed using Thermo Scientific™ TraceFinder™ software to ensure full automation from instrument setup to raw data collection, processing, and reporting. Data acquired from DIA were analyzed with an extraction mass tolerance of ≤5 ppm for both precursor and product ions. Analytes were quantified based on full scan data. In addition, confirmation of target pesticides was performed using DIA fragment matching against a curated, high-resolution spectral library. The Thermo Scientific™ AcquireX™ Background Exclusion workflow was applied, and the data was extracted with a mass tolerance of ≤5 ppm for both precursor and product ions. Analytes were first confirmed using a targeted list of pesticides from a compound database and matched with the spectral library. All unknown pesticides were automatically passed to the unknown workflow in TraceFinder software to search online compound databases as well as other local databases.

Results and discussion

Simplified in-house validation for screening and semi-quantitative methods was carried out on targeted pesticides. The linearity of the calibration curves was assessed over the range from 0.5 to 500 ng/mL to demonstrate the potential of the method for quantitative analysis. Method selectivity was evaluated by comparison of blank olive oil and spiked samples (n=6). The evaluation was based on accurate precursor *m/z* value of the analyte at the specified retention time window (±0.1 min). Full scan quantitation based upon mono-isotopic match, presence of fragment ions (FI), and high-resolution curated pesticide spectral library search (LS) was additionally applied for confirmation according to References 1 and 2. Acceptance values were set to less than or equal to 5 ppm for mass accuracy (FS and MS²), ± 0.1 min for retention time, reproducibility at LOQ ≤15%, at least one fragment ion present, and for passing LS matching a report out of greater than or equal to 60% and a *r*² ≥ 0.9000. The established values are shown in Table 2.

The methodology showed excellent reproducibility in terms of a) consistent peak shapes and robust column life, with over 250 injections and b) consistent peak response over time. Figure 1 shows select pesticides across the retention time range of the method (0–8 minutes), for 250 injections with a retention shift of less than 0.1 min. Figure 2 shows

a chromatogram of a 10 ppb matrix-matched standard (MMS) for a method containing over 500 pesticides with positive and negative polarity switching occurring throughout the run. Enough data points were obtained across each peak for accurate quantitation.

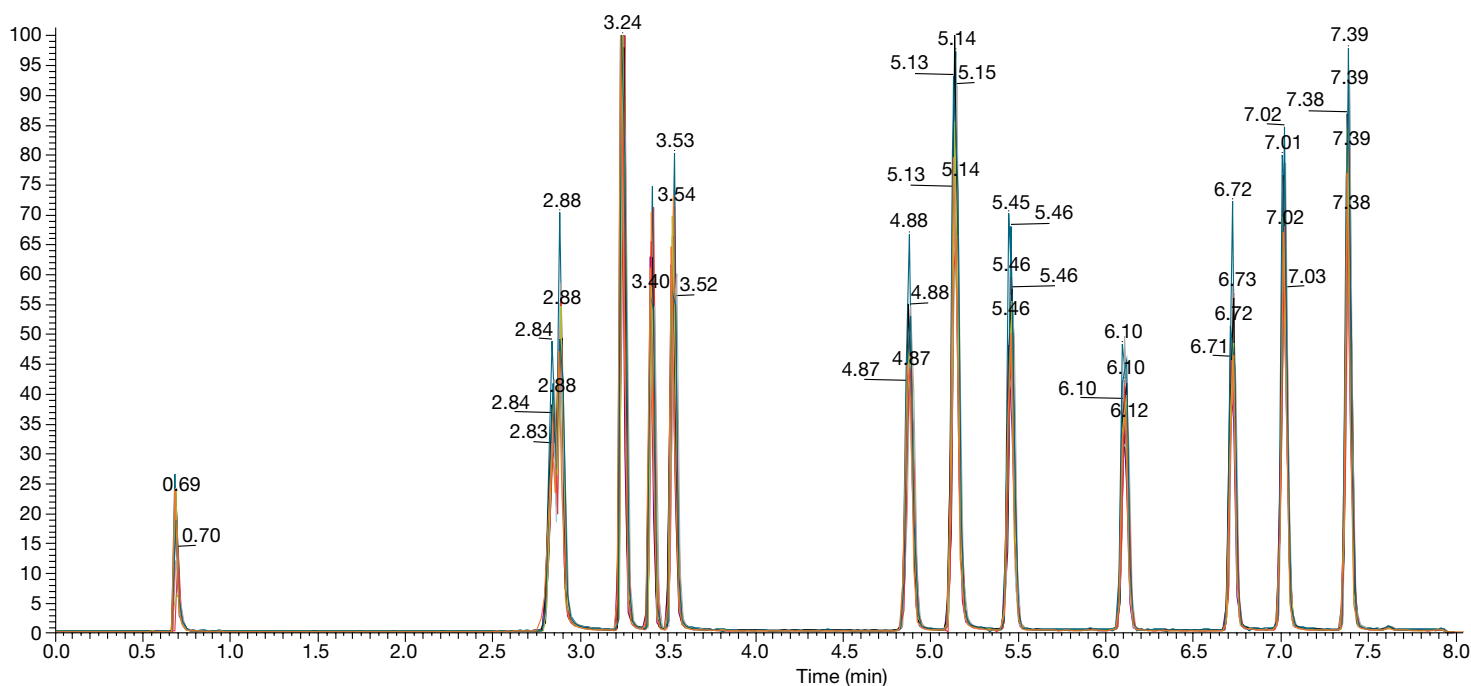


Figure 1. Robust LC-MS reproducibility of pesticides spiked in olive oil, selected pesticides (overlay of injections 1 to 250) with extracted mass tolerance of 3 ppm

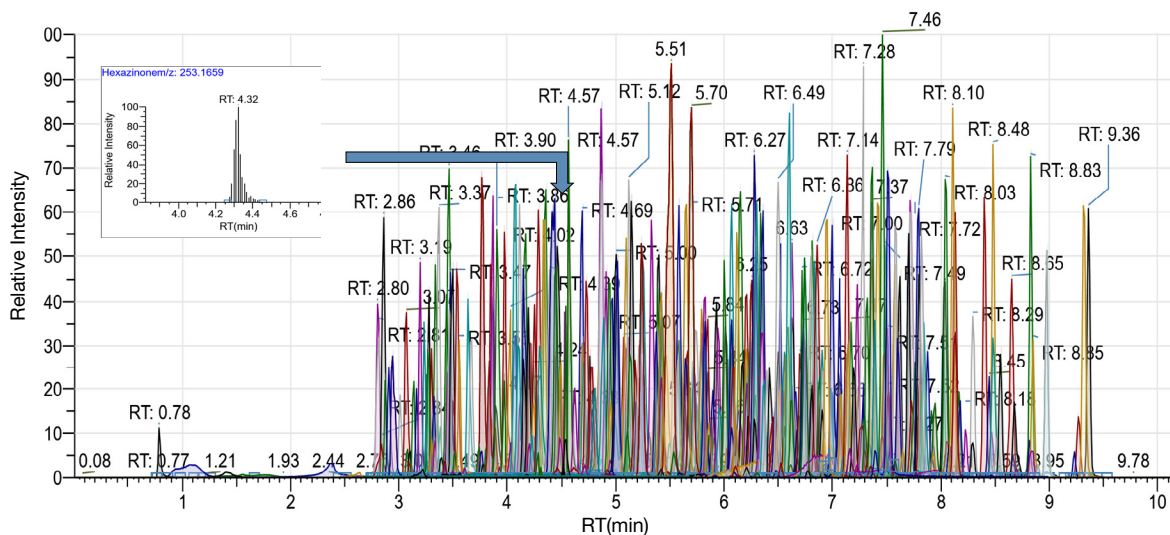


Figure 2. Chromatogram of over 500 pesticides in 15 min in olive oil MMS spiked at 10 ppb. The peak highlighted at 4.32 min is hexazinone showing over 11 scans across the Full Scan quantitation ion used for the analysis.

The implementation of the AcquireX Background Exclusion workflow also helps in identification of unknown contaminants using a unique routine to automatically create an exclusion list based on LC-MS analysis of the matrix blank. The instrument method is automatically updated with the exclusion list, so that when subsequent samples are analyzed, MS² experiments are not performed on matrix background signals. As a result, more cycle time is spent on triggering MS² on the relevant ions of interest. This is groundbreaking for data processing because

it is minimizing false positives and negatives. Utilizing TraceFinder software, these new acquired data files can be quickly used and data processing performed for known and unknown screening workflows. TraceFinder software can easily go from a known to an unknown workflow by simply selecting a check box (Figure 3). The software can be set to search multiple spectral libraries, along with online spectral databases such as ChemSpider by simply selecting the Exhaustive Search Feature option (Figure 4).

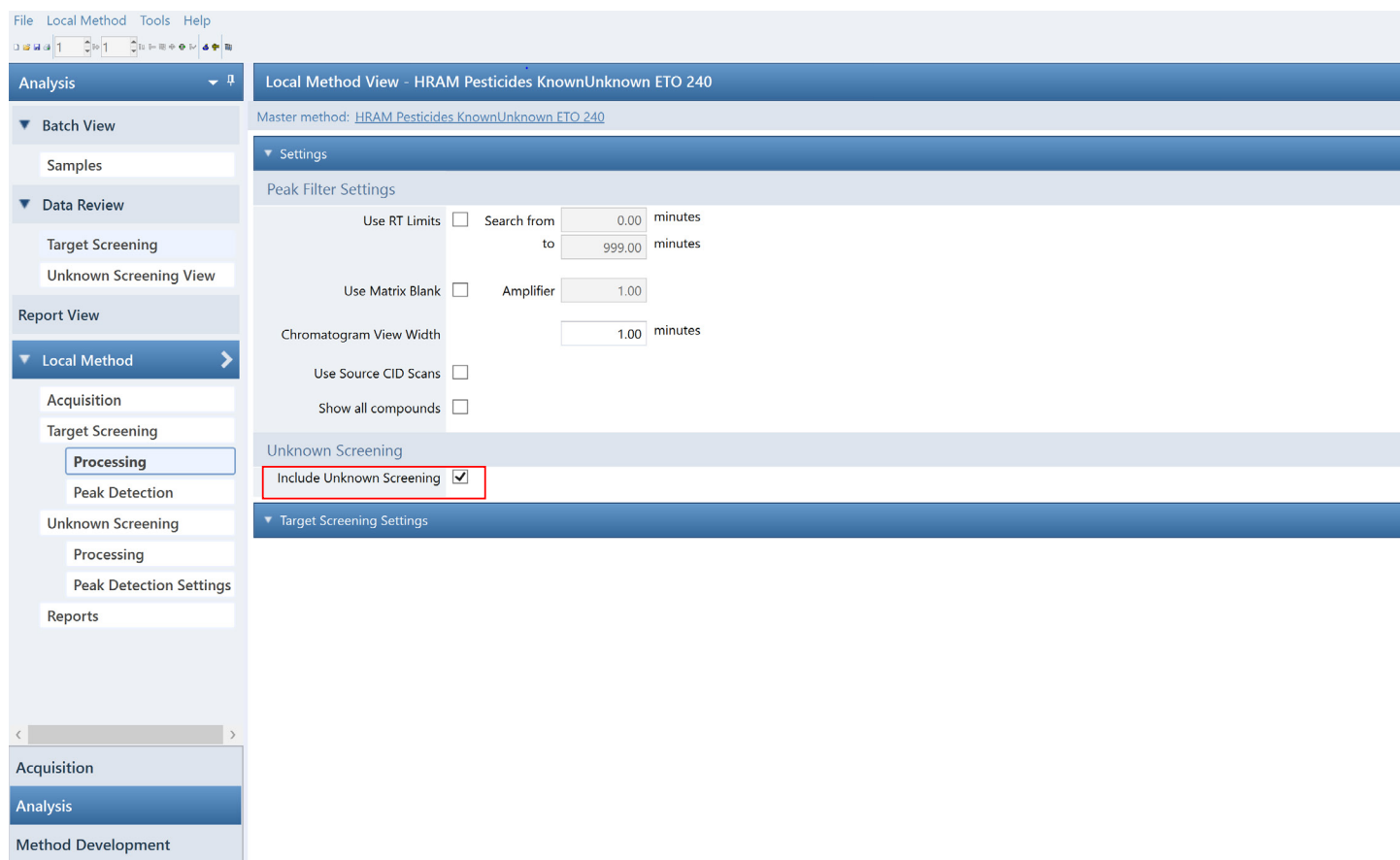


Figure 3. TraceFinder software easy configuration from known screening workflow to immediately activate unknown screening workflow with a check

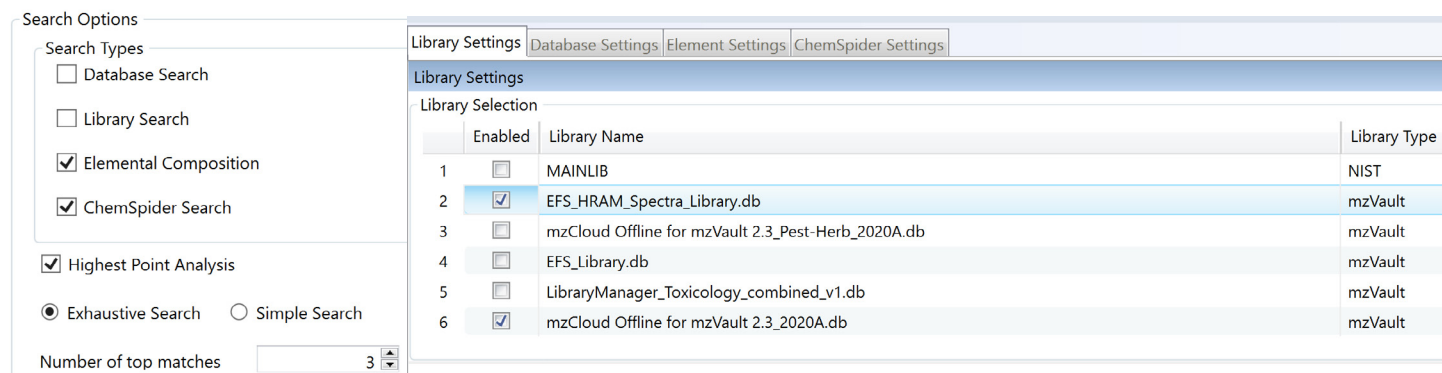


Figure 4. Unknown search parameters are easily activated by checking the box. The capability to search multiple localized mzCloud curated spectral libraries gives you the confidence of the exact match.

This feature ensures that the best results are displayed based on the search criteria selected. Figure 5 shows the quick and easy data review section of the targeted screening workflow with sortable grids and detailed information at the bottom. Chlorpyrifos (highlighted) is shown as an example of consistent mass measurement accuracy of the Orbitrap Exploris 240 mass spectrometer. Only those compounds that were not identified in the targeted screening workflow will be automatically moved into the unknown workflow for further investigation. An

example of this is shown in Figure 6 for compounds moved into the unknown screening workflow. In many cases, the ChemSpider database was used to identify and label the most likely hits with the corresponding elemental composition. Many unknowns were identified as fatty oil (oleic acid) chemicals from olive oil (e.g., palmitoleic acid and myristoleic acid). A unique compound called erucamide was also identified, and research shows that it is a “slip additive” that is most commonly used in plastics and was later used as lubricants (Figure 7).

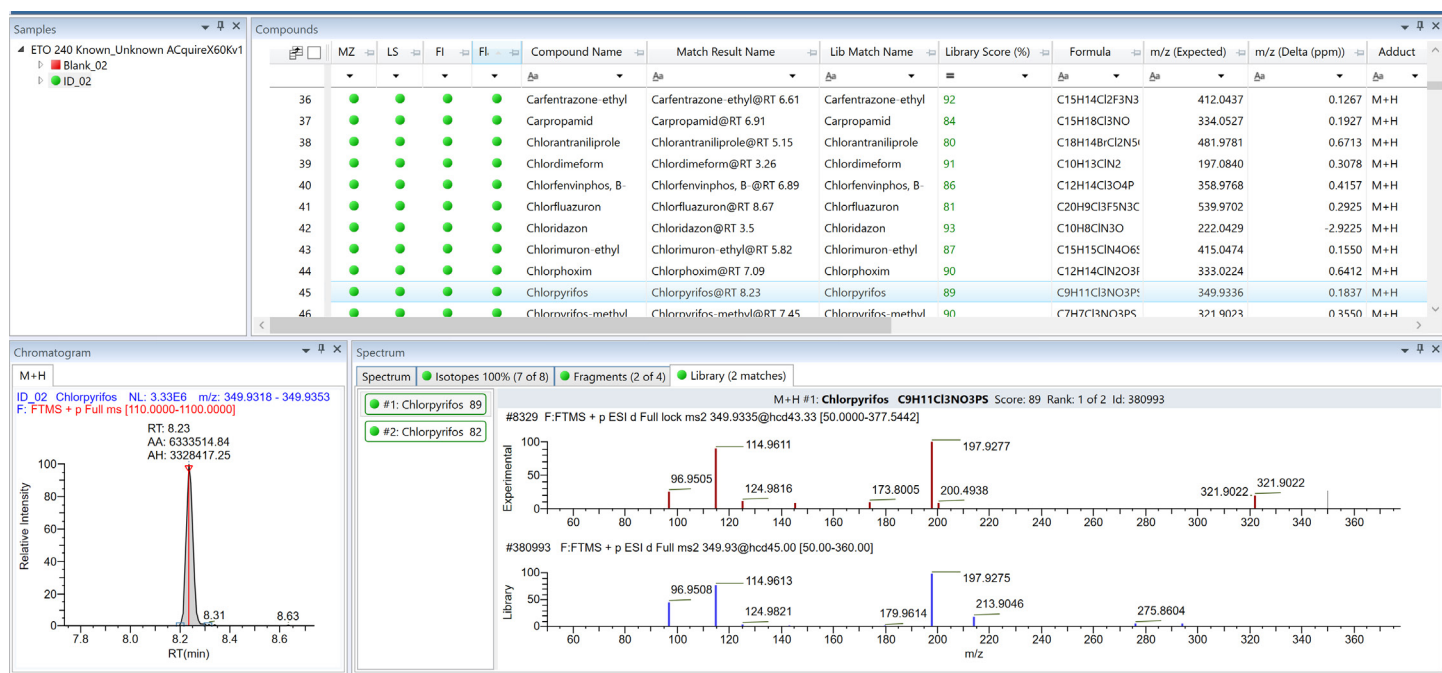


Figure 5. Quick overview of targeted compound detection for chlorpyrifos with library scoring of 89% and Δ ppm of 0.1837

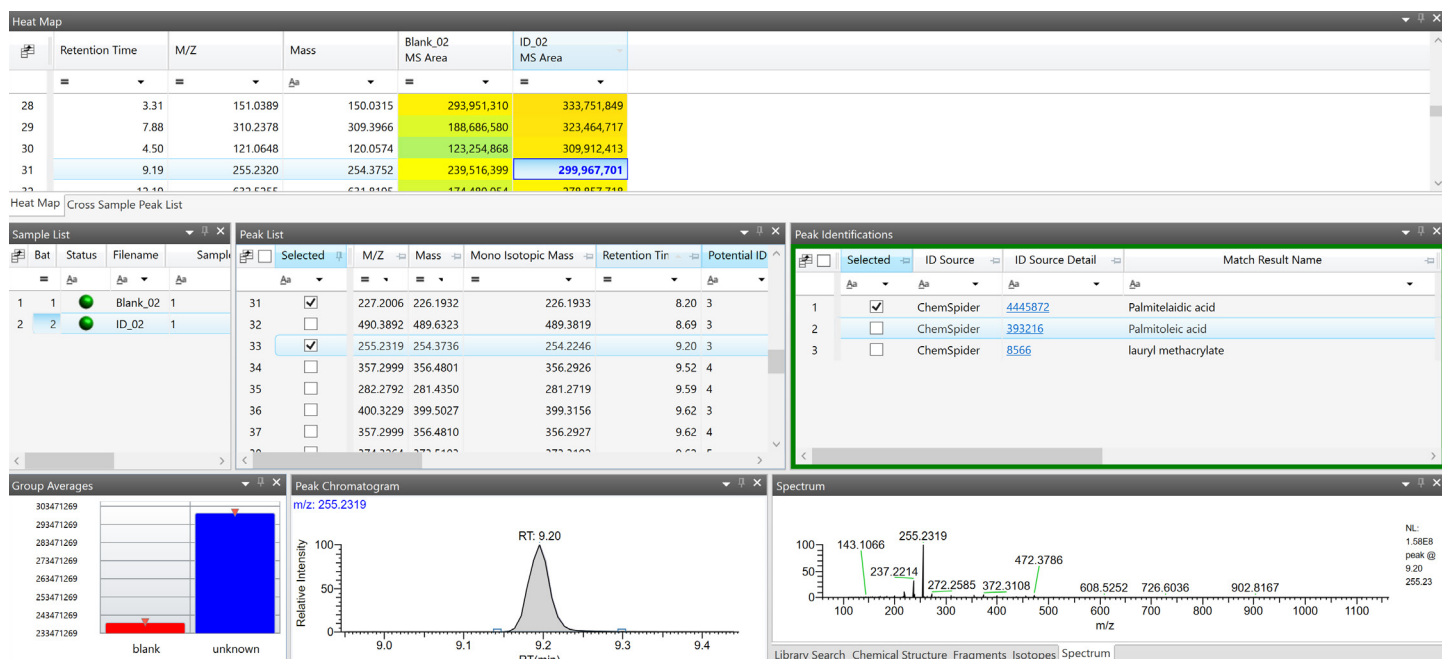


Figure 6. Quick overview of unknown screening where identification is quickly listed. Here is a highlighted example of palmitoleic acid found in the sample, a fatty acid in olive oil that was not being targeted.

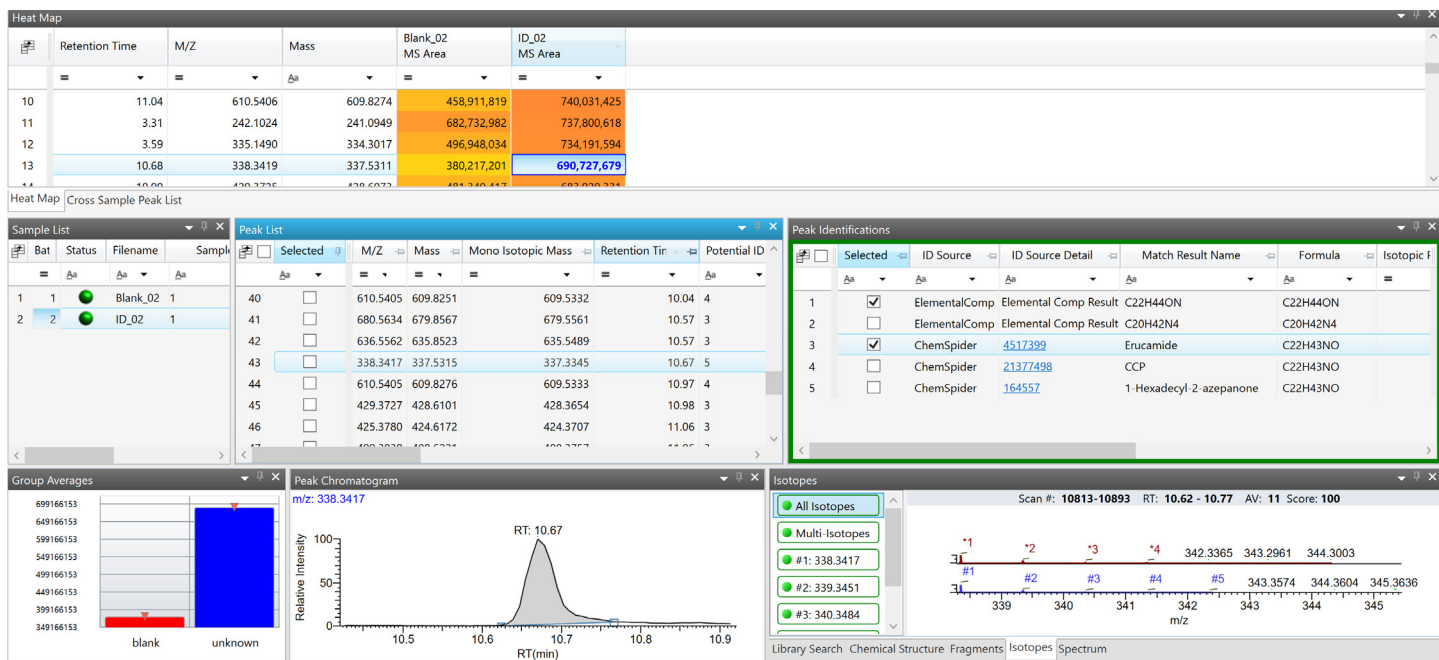


Figure 7. Quick overview of unknown screening that found enucamide, a lubricant in olive oil

Figure 8 shows calibration curves for ametryn and fenazaquin from 0.5 to 100 and 0.5 to 500 ppb, respectively. Over 95% of the pesticides studied had calibration curves with $r^2 > 0.950$ (Table 2). Confirmation fragment ions are displayed in the middle of each panel at 1 and 0.5 ppb for each pesticide, with indicator colors (green) easily visible to show passing fragment ion and

curated Thermo Scientific™ mzCloud™ local spectral library criteria. A polarity switching method of over 500 pesticides was developed and optimized to ensure that at least one fragment ion was detected per compound. LOQs were determined as outlined by the SANTE/11813/2017 guidelines, with results shown in Figure 9.



Figure 8. Quantitation ions and confirming ion in MMS in olive oil, along with calibration range from 0.5 to 100 (500) ppb in TraceFinder software for ametryn at 1 ppb and fenazaquin at 0.5 ppb, which shows excellent r^2 , MS² fragment ion matching. The technique allows for confident quantitation and screening with confirmation well below the MRL concentration.

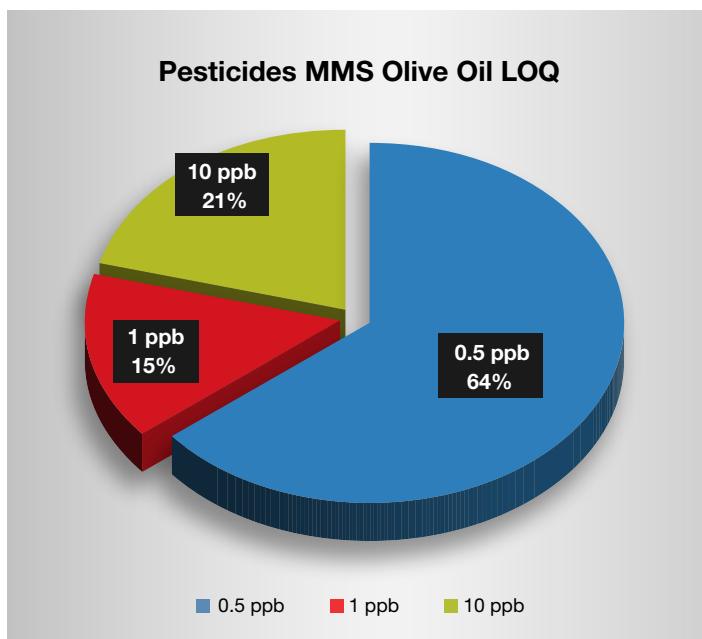


Figure 9. LOQs of pesticides in MMS in olive oil obtained following the SANTE guidelines for the screening method of over 400 pesticides

Conclusion

Large pesticide panels for quantitative analysis at levels at or below EU MRLs have been shown to provide excellent sensitivity and robustness in a routine laboratory setting for olive oil matrix. In addition, TraceFinder software gives you the flexibility to screen for unknown contaminants in the sample. The capability of searching online databases enables identification of unknowns due to the excellent mass accuracy and high resolving power of the Orbitrap Exploris 240 mass spectrometer, significantly lowering the number of extraneous ID possibilities. The new AcquireX Background Exclusion workflow, utilizing the automatic update of an instrument method with an exclusion list created from a blank matrix injection, allows elimination of unwanted background ions in MS² for real samples, making identification more reliable. Currently ongoing work is required to evaluate the performance of the residues in matrix extracted spikes (MES) extracts.

Acknowledgements

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References

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2. Acceptance Criteria for Confirmation of Identity of Chemical Residues using Exact Mass Data for the FDA FVM Program. *US Food & Drug Administration Office of Foods and Veterinary Medicine*. September 2015.

Table 2. Name of compound, r², concentration LOQ, RT, Δppm, %RSD, FI, and Library Score

Compound	R ²	LOQ conc. (ppb)	Actual RT (min)	Δ m/z (ppm)	%RSD	% CV	LS	FI	Library score (%)
2,6-Dichlorobenzamide	0.956	1.0	3.16	-0.555	10.01	6.07	Pass	Pass	100
Acephate	0.999	1.0	2.61	0.748	11.14	16.41	Pass	Pass	86
Acetamidrid	0.998	0.5	3.47	-0.372	9.22	8.79	Pass	Pass	95
Acetochlor	0.990	1.0	6.29	-0.267	9.65	11.84	Pass	Pass	98
Acibenzolar-S-methyl	0.996	1.0	6.28	-1.782	8.84	10.53	Pass	Pass	90
Alachlor	0.990	1.0	6.29	-0.267	9.65	11.84	Pass	Pass	98
Aldicarb-sulfoxide	0.998	0.5	2.84	-0.156	3.58	4.13	Pass	Pass	88
Allethrin	1.000	0.5	7.95	0.185	9.54	8.11	Pass	Pass	89
Ametryn	0.980	0.5	5.00	-0.172	4.35	4.81	Pass	Pass	87
Amicarbazone	0.999	10.0	4.04	0.181	6.87	7.18	Pass	Pass	90
Aminocarb	0.999	0.5	2.82	-0.372	3.49	4.05	Pass	Pass	96
Ancymidol	0.998	0.5	4.25	0.706	9.04	8.52	Pass	Pass	90
Anilofos	0.999	0.5	6.81	2.288	10.71	9.98	Pass	Pass	77
Aspon	0.999	0.5	8.48	0.029	3.84	3.88	Pass	Pass	92
Asulam	0.998	0.5	2.88	-0.282	2.95	2.62	Pass	Pass	100
Atrazine	0.999	0.5	4.87	-0.029	4.3	3.08	Pass	Pass	100
Azaconazole	0.999	0.5	5.23	0.341	4.54	4.49	Pass	Pass	86
Azamethiphos	0.998	0.5	4.03	0.553	7.86	5.95	Pass	Pass	84
Azinphos-ethyl	0.997	1.0	6.28	-0.199	5.24	5.42	Pass	Pass	86
Azinphos-methyl	0.998	10.0	5.38	1.380	6.71	6.28	Pass	Pass	90
Aziprotryne	0.999	0.5	5.93	0.493	1.17	1.59	Pass	Pass	82
Azoxystrobin	0.999	0.5	5.39	-0.341	2.29	2.5	Pass	Pass	100
Barban	0.994	10.0	5.94	-0.036	13.46	12.15	Pass	Pass	62
Beflubutamid	0.999	0.5	6.74	0.117	2.71	2.23	Pass	Pass	86
Benalaxyl	0.999	0.5	6.84	-0.159	5.67	6.04	Pass	Pass	98
Bendiocarb	0.999	0.5	4.17	0.094	4.56	3.74	Pass	Pass	99
Benodanil	0.998	1.0	4.79	-0.295	13.82	11.99	Pass	Pass	66
Benoxacor	0.999	0.5	5.31	0.807	9.73	9.97	Pass	Pass	85
Bensulide	0.999	0.5	6.55	-0.155	6.18	5.01	Pass	Pass	93
Benthiavalicarb-isopropyl	0.998	0.5	5.82	-0.411	4.48	4.34	Pass	Pass	88
Benzofenap	0.999	0.5	7.62	0.086	2.63	2.54	Pass	Pass	95
Benzoylprop-ethyl	0.998	0.5	6.91	-0.343	5.95	4.87	Pass	Pass	98
Bioresmethrin	0.999	0.5	8.98	-0.194	4.85	4.62	Pass	Pass	88
Boscalid	0.998	0.5	5.71	-1.224	5.2	4.68	Pass	Pass	100
Brodifacoum	1.000	0.5	9.27	1.171	7.84	7.64	Pass	Pass	86
Bromacil	0.997	0.5	4.19	0.918	12.99	13.41	Pass	Pass	97
Bromfenvinphos-ethyl	0.999	0.5	6.99	-0.430	5.39	5.28	Pass	Pass	85
Bupirimate	0.999	0.5	6.15	0.079	3.77	4.65	Pass	Pass	93
Buprofezin	0.998	0.5	7.79	0.273	2.16	2.65	Pass	Pass	96
Butachlor	0.974	100.0	8.00	0.017	12.62	11.61	Pass	Pass	91
Butafenacil_M+NH4	0.999	0.5	6.04	0.144	5	4.24	Pass	Pass	88
Butralin	0.999	0.5	8.47	0.556	7.06	7.87	Pass	Pass	90
Buturon	0.997	0.5	4.97	0.766	4.18	3.55	Pass	Pass	87
Butylate	0.999	1.0	7.65	-1.082	10.05	15.49	Pass	Pass	93

Table 2. Name of compound, r², concentration LOQ, RT, Δppm, %RSD, FI, and Library Score

Compound	R ²	LOQ conc. (ppb)	Actual RT (min)	Δ m/z (ppm)	%RSD	% CV	LS	FI	Library score (%)
Carbendazim	0.999	0.5	3.19	0.406	6.78	6.57	Pass	Pass	95
Carbetamide	0.998	0.5	3.96	0.890	12.84	13.56	Pass	Pass	97
Carbofuran	0.998	1.0	4.16	0.011	11.18	9.56	Pass	Pass	100
Carbofuran, 3OH-	0.998	0.5	3.38	0.945	5.62	5.07	Pass	Pass	96
Carboxin	0.997	1.0	4.46	-0.281	3.47	2.39	Pass	Pass	91
Carfentrazone-ethyl	0.994	0.5	6.60	-0.021	9.41	7.1	Pass	Pass	95
Carpropamid	0.999	0.5	6.90	-0.447	5.07	4.5	Pass	Pass	93
Chlorantraniliprole	0.997	1.0	5.15	-1.798	10.59	9.87	Pass	Pass	83
Chlorbromuron	0.999	0.5	5.90	0.622	2.43	2.3	Pass	Pass	85
Chlorfenvinphos, B-	0.998	0.5	6.89	0.246	5.08	5.35	Pass	Pass	86
Chlorfluazuron	0.998	10.0	8.65	0.745	3.51	3.37	Pass	Pass	74
Chloridazon	0.988	10.0	3.49	-2.098	8.33	5.84	Pass	Pass	96
Chlorimuron-ethyl	0.998	0.5	5.80	-0.360	3.29	3.27	Pass	Pass	87
Chloroxuron	0.999	0.5	6.20	-0.009	4.59	4.14	Pass	Pass	85
Chlorphoxim	0.999	0.5	7.08	0.458	6.79	5.76	Pass	Pass	92
Chlorpyrifos	0.999	0.5	8.23	0.358	6.25	4.99	Pass	Pass	91
Chlorpyrifos-methyl	0.998	10.0	7.44	-0.119	8.11	8.39	Pass	Pass	100
Chlorsulfuron	0.998	0.5	4.38	1.647	10.28	9.73	Pass	Pass	84
Chlortoluron	0.998	0.5	4.88	-0.509	5.56	4.31	Pass	Pass	95
Cinidon-ethyl	0.999	0.5	8.08	-0.645	8.32	8.76	Pass	Pass	73
Cinosulfuron	0.991	100.0	3.90	0.266	8.85	8.28	Pass	Pass	90
Clethodim	0.997	0.5	7.52	-0.098	5.32	3.29	Pass	Pass	83
Clodinafop-propargyl	0.997	0.5	6.60	-0.086	6.37	4.5	Pass	Pass	92
Clofentezine	0.988	0.5	7.51	0.058	12.5	4.56	Pass	Pass	79
Clomazone	1.000	0.5	5.37	-0.688	2.22	2.2	Pass	Pass	100
Cloquintocet-mexyl	0.999	0.5	8.13	0.116	5.62	6.37	Pass	Pass	96
Clothianidin	0.998	10.0	3.32	0.148	6.82	6.64	Pass	Pass	89
Coumaphos	0.999	1.0	6.98	0.221	13.38	13.35	Pass	Pass	89
Coumatetralyl	0.997	0.5	6.27	0.306	5.71	4.24	Pass	Pass	97
Crimidine	0.998	1.0	3.86	1.500	5.88	7.99	Pass	Pass	89
Cumyluron	0.998	0.5	6.06	-0.353	1.21	0.94	Pass	Pass	95
Cyanazine	0.998	1.0	3.97	0.436	9.32	8.35	Pass	Pass	100
Cyazofamid	0.998	0.5	6.36	0.228	4.38	3.1	Pass	Pass	85
Cyclanilide	0.993	10.0	6.37	0.463	4.99	4.79	Pass	Pass	86
Cycloate	0.999	0.5	7.39	-0.835	4.09	5.21	Pass	Pass	94
Cyclosulfamuron	0.999	0.5	6.20	-0.206	4.05	3.72	Pass	Pass	93
Cycloxydim	0.999	0.5	7.58	-0.011	2.46	2.03	Pass	Pass	88
Cycluron	0.999	1.0	5.15	-0.735	10.8	9.85	Pass	Pass	98
Cyflufenamid	0.996	0.5	7.05	-0.453	7.05	3.67	Pass	Pass	84
Cyprazine	0.998	0.5	4.88	0.574	5.14	3.48	Pass	Pass	84
Cyproconazole	0.998	0.5	5.85	0.537	9.3	8.13	Pass	Pass	98
Cyprodinil	0.998	0.5	6.86	0.519	2.65	3.27	Pass	Pass	100
Cyromazine	1.000	1.0	2.37	-2.810	1.61	3.57	Pass	Pass	89
DEF	1.000	0.5	8.83	0.240	4.91	4.51	Pass	Pass	92

Table 2. Name of compound, r², concentration LOQ, RT, Δppm, %RSD, FI, and Library Score

Compound	R ²	LOQ conc. (ppb)	Actual RT (min)	Δ m/z (ppm)	%RSD	% CV	LS	FI	Library score (%)
Demeton	0.998	0.5	5.33	3.039	7.06	10.07	Pass	Pass	97
Demeton-S (disulfoton oxon)	0.998	0.5	5.33	3.039	7.06	10.07	Pass	Pass	86
Demeton-S-methyl-sulfone	0.997	1.0	3.10	-0.037	7.89	7.97	Pass	Pass	84
Desmetryn	0.999	0.5	4.44	-0.066	4.06	4.17	Pass	Pass	92
Diafenthiuron	0.998	1.0	8.52	0.699	3.67	5.46	Pass	Pass	78
Dialifor	0.999	0.5	7.28	-0.062	4.96	4.59	Pass	Pass	88
Diallate	0.995	100.0	7.46	-1.826	6.99	6.49	Pass	Pass	78
Dibutyl phthalate	0.998	10.0	7.51	-0.007	4.52	2.68	Pass	Pass	87
Dibutyl succinate	0.999	10.0	6.70	0.256	2.8	2.67	Pass	Pass	99
Dichlofluanid	0.984	100.0	6.15	2.090	9.08	8.25	Pass	Pass	89
Dichlorvos	0.999	0.5	4.21	1.132	7.5	10.47	Pass	Pass	87
Diclobutrazol	0.999	0.5	6.66	-0.780	5.4	4.94	Pass	Pass	88
Diclosulam	0.988	10.0	4.48	-0.338	5.57	5.48	Pass	Pass	83
Diethyl toluamide	0.995	1.0	4.92	-0.554	14.95	7.33	Pass	Pass	90
Difenacoum	0.999	0.5	8.66	0.594	7.46	7.14	Pass	Pass	94
Difenoconazole	0.999	0.5	7.41	0.427	8.09	6.54	Pass	Pass	100
Difenoxuron	0.999	0.5	5.10	0.488	5.27	4.54	Pass	Pass	87
Diflubenzuron	0.999	0.5	6.67	0.285	9.27	6.72	Pass	Pass	95
Diflufenican	0.997	10.0	7.56	-0.284	11.58	9.18	Pass	Pass	100
Dimefuron	0.999	0.5	5.18	-1.841	7.97	5.94	Pass	Pass	97
Dimepiperate	0.997	0.5	7.45	0.356	5.6	9.5	Pass	Pass	88
Dimethachlor	0.997	0.5	5.12	0.292	4.25	3.93	Pass	Pass	100
Dimethametryn	0.998	0.5	6.28	0.188	2.3	2.99	Pass	Pass	88
Dimethenamid	0.998	0.5	5.57	-0.037	1.16	1.21	Pass	Pass	100
Dimethirimol	0.998	0.5	3.76	0.460	7.67	8.1	Pass	Pass	92
Dimethoate	0.997	0.5	3.45	-0.146	6.38	5.07	Pass	Pass	97
Dimethomorph	0.997	0.5	5.79	-0.152	8.99	6.12	Pass	Pass	97
Diniconazole	0.999	0.5	7.29	0.696	3.85	3.37	Pass	Pass	93
Dinotefuran	0.999	0.5	2.91	-0.194	6.61	6.6	Pass	Pass	87
Dioxacarb	0.997	0.5	3.41	-2.561	1.72	1.61	Pass	Pass	89
Diphenamid	0.998	0.5	5.13	-1.142	5.4	5.4	Pass	Pass	87
Dipropetryn	0.998	0.5	6.28	0.188	2.3	2.99	Pass	Pass	81
Disulfoton sulfone	0.998	0.5	4.73	0.079	2.67	2.5	Pass	Pass	89
Dithiopyr	0.996	0.5	7.52	-0.497	9.91	5.72	Pass	Pass	84
Diuron	0.998	0.5	5.24	0.991	3.02	2.28	Pass	Pass	100
DMST	0.999	0.5	4.28	-0.358	4.02	3.83	Pass	Pass	97
Dodemorph	0.999	1.0	5.09	0.123	4.67	4.75	Pass	Pass	91
Dodine	0.999	0.5	7.29	0.015	7.94	10.61	Pass	Pass	93
D-Trans-allethrin	1.000	0.5	7.95	0.185	9.54	8.11	Pass	Pass	93
Edifenphos	0.998	0.5	6.81	0.684	8.81	6.63	Pass	Pass	81
Emamectin benzoate	0.999	0.5	8.04	0.766	4.29	5.4	Pass	Pass	88
Epoxiconazole	0.999	0.5	6.39	0.072	6.87	5.15	Pass	Pass	99
EPTC	0.999	1.0	6.62	-1.139	5.78	9.22	Pass	Pass	87
Ethiofencarb	0.986	0.5	4.54	-0.944	11.83	10.26	Pass	Pass	88

Table 2. Name of compound, r², concentration LOQ, RT, Δppm, %RSD, FI, and Library Score

Compound	R ²	LOQ conc. (ppb)	Actual RT (min)	Δ m/z (ppm)	%RSD	% CV	LS	FI	Library score (%)
Ethion	1.000	0.5	8.02	-0.282	0.55	0.5	Pass	Pass	92
Ethiprole	0.998	0.5	5.55	-0.003	2.77	2.56	Pass	Pass	83
Ethirimol	0.998	0.5	3.76	0.460	7.67	8.1	Pass	Pass	84
Ethofumesate	0.998	0.5	5.44	-0.258	5.77	4.46	Pass	Pass	93
Ethoprophos	0.998	0.5	6.28	0.168	2.71	2.6	Pass	Pass	92
Ethoxyquin	0.998	0.5	4.85	0.307	5.94	8.99	Pass	Pass	93
Etofenprox	0.999	0.5	9.37	0.235	3.75	3.91	Pass	Pass	91
Etoxazole	1.000	0.5	8.40	0.032	3.88	4.27	Pass	Pass	95
Fenamidone	0.998	0.5	5.54	0.020	4.55	4.61	Pass	Pass	90
Fenamiphos	0.999	0.5	6.50	0.662	5.88	5.08	Pass	Pass	84
Fenamiphos-sulfone	0.998	1.0	4.25	0.440	5.67	5.2	Pass	Pass	73
Fenamiphos-sulfoxide	0.999	0.5	4.16	-0.059	8.3	6.38	Pass	Pass	74
Fenarimol	0.990	0.5	6.20	-0.438	8.01	3.61	Pass	Pass	90
Fenazaquin	0.994	0.5	9.32	-0.427	2.44	1.78	Pass	Pass	87
Fenbuconazole	0.998	0.5	6.44	-0.423	6.12	4.37	Pass	Pass	92
Fenfuram	0.938	1.0	4.55	-0.992	5.54	2.93	Pass	Pass	97
Fenhexamid	0.988	1.0	6.06	0.346	4.05	2.73	Pass	Pass	95
Fenoxanil	0.999	0.5	6.45	-0.255	4.94	4.46	Pass	Pass	89
Fenoxycarb	0.997	0.5	6.59	-0.229	5.79	3.58	Pass	Pass	97
Fenpropidin	0.999	0.5	5.25	-0.669	4.87	5.24	Pass	Pass	100
Fenpropimorph	0.999	0.5	5.41	0.698	2.59	2.92	Pass	Pass	100
Fenpyroximate	0.999	0.5	8.64	0.574	3.46	3.4	Pass	Pass	100
Fensulfothion	0.998	10.0	4.95	0.731	6.75	6.64	Pass	Pass	85
Fenthion	0.998	1.0	6.92	0.813	7.13	7.04	Pass	Pass	65
Fenthion-sulfoxide	0.998	0.5	4.39	-0.184	10.1	8.03	Pass	Pass	84
Fentrazamide	0.998	1.0	6.80	-1.866	8.78	8.35	Pass	Pass	95
Fenuron	0.998	0.5	3.46	-0.314	2.95	3.01	Pass	Pass	96
Flamprop Isopropyl	0.997	0.5	6.83	-0.271	7.41	5.02	Pass	Pass	84
Flamprop-methyl	0.999	0.5	5.94	-0.235	2.43	2.53	Pass	Pass	80
Fluazifop-butyl	0.998	0.5	7.71	0.248	4.41	4.05	Pass	Pass	98
Fluazifop-P-butyl	0.998	0.5	7.71	0.248	4.41	4.05	Pass	Pass	98
Fluazuron	0.999	0.5	8.16	-0.349	4.04	3.74	Pass	Pass	92
Flufenacet	0.998	0.5	6.20	-0.362	6.28	5.16	Pass	Pass	97
Flumetsulam	0.997	0.5	3.32	-1.004	9.95	6.99	Pass	Pass	92
Fluometuron	0.998	0.5	4.68	0.305	5.08	4.62	Pass	Pass	94
Fluopyram	0.998	0.5	6.07	-0.332	3.69	2.89	Pass	Pass	88
Fluoxastrobin	0.999	0.5	6.06	0.219	6.62	5.42	Pass	Pass	95
Fluridone	0.999	0.5	5.33	0.050	3.11	3.25	Pass	Pass	87
Fluroxypyr	0.987	500.0	3.96	0.793	1.46	1.41	Pass	Pass	94
Flurtamone	0.997	0.5	5.59	-0.062	2.71	2.82	Pass	Pass	97
Flusilazole	0.998	0.5	6.56	0.467	4.42	3.48	Pass	Pass	97
Fluthiacet-methyl	1.000	0.5	6.76	-0.053	2.47	2.3	Pass	Pass	85
Flutolanil	0.998	0.5	5.78	-0.046	6.09	5.22	Pass	Pass	98
Flutriafol	0.999	0.5	4.79	-1.701	8.33	7.35	Pass	Pass	90

Table 2. Name of compound, r², concentration LOQ, RT, Δppm, %RSD, FI, and Library Score

Compound	R ²	LOQ conc. (ppb)	Actual RT (min)	Δ m/z (ppm)	%RSD	% CV	LS	FI	Library score (%)
Fluxapyroxad	0.996	0.5	5.82	-0.105	5.73	3.42	Pass	Pass	86
Forchlorfenuron	0.998	0.5	5.13	-0.871	8.63	8.62	Pass	Pass	94
Fosthiazate	0.985	0.5	4.60	-0.060	6.98	6.4	Pass	Pass	89
Fuberidazole	0.998	0.5	3.45	-0.505	3.67	3.58	Pass	Pass	88
Furalaxyl	0.998	0.5	5.42	-0.330	2.58	2.37	Pass	Pass	97
Furathiocarb	0.998	0.5	7.73	-0.177	3.34	3.45	Pass	Pass	89
Griseofulvin	0.998	0.5	4.79	0.529	5.89	5.01	Pass	Pass	61
Halofenozide	0.996	10.0	5.60	-0.066	4.2	3.91	Pass	Pass	84
Haloxyfop-2-ethoxyethyl	0.998	0.5	7.63	-0.501	2.43	2.55	Pass	Pass	89
Heptenophos	0.999	0.5	5.10	0.437	3.8	3.44	Pass	Pass	91
Hexaconazole	0.999	0.5	7.01	-0.152	5.85	4.47	Pass	Pass	91
Hexazinone	0.957	0.5	4.30	0.155	7.93	4.97	Pass	Pass	97
Hexythiazox	0.999	0.5	8.18	0.750	5.87	5.52	Pass	Pass	97
Hydramethylnon	0.998	0.5	7.49	0.050	8.91	7.2	Pass	Pass	86
Imazalil	0.998	0.5	4.70	-0.298	4.47	5.32	Pass	Pass	88
Imazamox	0.997	0.5	3.47	-0.976	6.27	6.36	Pass	Pass	100
Imazapic	0.999	0.5	3.53	-0.637	6.02	5.6	Pass	Pass	89
Imazaquin	0.998	0.5	4.16	0.024	7.48	6.41	Pass	Pass	98
Imidacloprid	0.961	100.0	3.30	0.558	4.82	4.45	Pass	Pass	96
Inabenfide	0.997	0.5	5.60	-0.457	4.35	3.41	Pass	Pass	84
Indoxacarb	0.999	0.5	7.34	0.140	7.22	5.29	Pass	Pass	82
Ipconazole	0.995	0.5	7.52	0.245	6.79	3.67	Pass	Pass	90
Iprobenfos	0.998	0.5	6.64	-0.130	3.81	4.21	Pass	Pass	97
Iprovalicarb	0.999	0.5	6.14	0.332	4.11	4.4	Pass	Pass	96
Isazofos	0.997	0.5	6.00	0.098	2.01	2.36	Pass	Pass	96
Isomethiozin	0.999	0.5	6.80	1.158	3.7	3.59	Pass	Pass	94
Isoprocab	0.999	100.0	4.80	-1.054	2.97	2.8	Pass	Pass	97
Isoprothiolane	0.999	0.5	5.84	-0.000	1.56	1.97	Pass	Pass	86
Isoproturon	0.999	0.5	5.00	0.050	6.29	5.72	Pass	Pass	95
Isopyrazam	0.999	0.5	7.37	-0.079	8.9	7.74	Pass	Pass	89
Isouron	0.997	0.5	4.37	0.112	7.74	7.66	Pass	Pass	91
Isoxadifen-ethyl	0.995	0.5	6.60	0.079	4.28	2.78	Pass	Pass	79
Isoxaflutole	0.997	10.0	4.91	0.390	12.1	10.67	Pass	Pass	90
Isoxathion	0.998	0.5	7.14	0.665	2.75	2.96	Pass	Pass	89
Kadethrin	0.998	0.5	7.50	0.179	15	14.77	Pass	Pass	89
Kresoxim-methyl	0.998	0.5	6.62	0.071	4.57	4.72	Pass	Pass	84
Lactofen	0.998	0.5	7.82	-0.588	13.42	9.55	Pass	Pass	85
Lenacil	0.994	10.0	4.93	1.250	5.33	5.32	Pass	Pass	100
Linuron	0.999	0.5	5.72	0.432	5.06	4.78	Pass	Pass	97
Malathion	0.998	0.5	5.82	-0.661	3.14	3.55	Pass	Pass	88
Mandipropamid	0.996	0.5	5.67	0.301	7.9	5.67	Pass	Pass	91
Mecarbam	0.999	0.5	6.20	-0.289	3.44	3.32	Pass	Pass	92
Mefenpyr-diethyl	0.998	0.5	6.91	-0.368	5.76	6.1	Pass	Pass	97
Mefluidide	0.997	0.5	4.21	0.880	7.3	5.11	Pass	Pass	85

Table 2. Name of compound, r², concentration LOQ, RT, Δppm, %RSD, FI, and Library Score

Compound	R ²	LOQ conc. (ppb)	Actual RT (min)	Δ m/z (ppm)	%RSD	% CV	LS	FI	Library score (%)
Mepanipyrim	0.999	0.5	6.49	0.431	2.31	3.04	Pass	Pass	91
Mephospholan	0.997	0.5	4.07	0.369	8.23	8.06	Pass	Pass	83
Mepronil	0.999	0.5	5.84	-0.095	1.96	1.72	Pass	Pass	87
Metaflumizone	0.998	1.0	7.92	-0.280	12.23	13.22	Pass	Pass	75
Metalaxyl	0.999	0.5	4.87	-0.227	3.8	3.44	Pass	Pass	97
Metalaxyl-M	0.999	0.5	4.87	-0.227	3.8	3.44	Pass	Pass	97
Metamitron	0.984	100.0	3.51	-0.436	11	4.66	Pass	Pass	98
Metazachlor	0.998	0.5	4.86	0.544	6.22	6.89	Pass	Pass	95
Metconazole	0.998	0.5	7.05	-0.429	3.04	2.13	Pass	Pass	96
Methabenzthiazuron	0.999	0.5	5.21	-0.528	2.69	2.65	Pass	Pass	82
Methacrifos	0.999	10.0	5.22	-0.153	4.83	5.91	Pass	Pass	85
Methamidophos	1.000	1.0	1.80	-0.888	3.87	4.46	Pass	Pass	80
Methfuroxam	0.998	0.5	5.24	0.503	2.3	2.29	Pass	Pass	98
Methiocarb	0.999	0.5	5.64	-1.012	3.41	3.26	Pass	Pass	90
Methiocarb-sulfone	0.992	1.0	3.46	0.503	10.77	5.29	Pass	Pass	88
Methiocarb-sulfoxide	0.998	1.0	3.33	2.873	8.3	9.58	Pass	Pass	98
Methomyl	0.989	10.0	3.09	-0.446	2.91	5.94	Pass	Pass	98
Methoxyfenozide	0.998	0.5	5.90	-0.207	5.95	7.15	Pass	Pass	100
Metobromuron	0.998	0.5	4.96	-0.157	8.21	7.43	Pass	Pass	90
Metolachlor	1.000	0.5	6.36	-0.020	2.79	2.94	Pass	Pass	100
Metolcarb	0.998	10.0	4.00	-0.564	10.45	9.78	Pass	Pass	96
Metosulam	0.997	0.5	4.25	-0.038	10.67	10.16	Pass	Pass	87
Metoxuron	0.996	0.5	3.84	-0.101	6.71	5.85	Pass	Pass	92
Metrafenone	0.999	0.5	7.20	0.383	3.65	3.53	Pass	Pass	99
Mexacarbate	0.999	0.5	3.40	-4.222	11.59	14.79	Pass	Pass	82
Molinate	0.998	0.5	6.09	-0.532	5.16	7.46	Pass	Pass	96
Monalide	0.997	0.5	6.42	0.021	2.34	2.31	Pass	Pass	96
Monolinuron	0.998	0.5	4.71	0.008	5.77	5.63	Pass	Pass	91
Monuron	0.998	0.5	4.26	0.578	7.25	6.04	Pass	Pass	100
Myclobutanil	0.999	0.5	5.95	0.140	3.14	3	Pass	Pass	83
Naled	0.997	10.0	5.09	1.949	12.6	11.03	Pass	Pass	84
Napropamide	0.999	0.5	6.33	0.935	3.61	4.13	Pass	Pass	99
Nicotine	0.994	1.0	0.79	-0.245	10.54	6.05	Pass	Pass	95
Novaluron	0.996	1.0	7.64	-0.243	2.83	2.61	Pass	Pass	95
Nuarimol	0.999	0.5	5.50	-0.521	4.46	4.2	Pass	Pass	89
Ofurace	0.997	0.5	4.17	0.188	9.42	8.86	Pass	Pass	69
Omethoate	0.999	0.5	2.82	-0.431	3.91	4.47	Pass	Pass	93
Orbencarb	0.999	10.0	7.15	0.318	3.69	3.77	Pass	Pass	97
Oxadiazon	0.998	0.5	7.93	0.269	7.74	6.66	Pass	Pass	93
Oxadixyl	0.996	0.5	3.83	0.698	7.82	8.28	Pass	Pass	84
Oxamyl	0.999	10.0	2.99	-0.309	2.84	3.19	Pass	Pass	88
Oxycarboxin	0.997	1.0	3.56	0.578	11.93	9.96	Pass	Pass	82
Oxydemeton methyl	0.999	0.5	3.06	0.275	8.39	8.91	Pass	Pass	84
Paclobutrazol	0.999	0.5	5.77	0.033	6.24	4.92	Pass	Pass	92

Table 2. Name of compound, r², concentration LOQ, RT, Δppm, %RSD, FI, and Library Score

Compound	R ²	LOQ conc. (ppb)	Actual RT (min)	Δ m/z (ppm)	%RSD	% CV	LS	FI	Library score (%)
Parathion-methyl-oxon	0.992	100.0	3.92	0.534	6.63	4.93	Pass	Pass	85
Parathion-oxon	0.998	10.0	4.79	0.741	9	8.49	Pass	Pass	89
Pebulate	0.999	0.5	7.27	0.536	6.46	7.28	Pass	Pass	92
Penconazole	0.996	0.5	6.83	-0.057	7.92	4.46	Pass	Pass	94
Pencycuron	0.999	0.5	7.24	0.062	3.03	3.22	Pass	Pass	96
Phenothrin	0.987	10.0	9.25	0.421	11.46	7.68	Pass	Pass	62
Phenthoate	0.998	0.5	6.62	0.229	5.54	4.85	Pass	Pass	94
Phorate	0.996	10.0	7.14	0.861	14.41	13.9	Pass	Pass	85
Phorate-sulfone	0.999	0.5	4.77	1.314	8.1	7.31	Pass	Pass	86
Phosalone	0.998	0.5	7.14	0.251	4.31	3.52	Pass	Pass	93
Phosfolan	0.999	1.0	3.73	-0.348	8.12	8.46	Pass	Pass	80
Phosmet	0.996	0.5	5.41	-0.030	13.6	3.54	Pass	Pass	98
Phoxim	0.998	1.0	7.08	0.786	13.4	7.07	Pass	Pass	92
Picolinafen	0.998	1.0	8.12	0.133	5.13	3.28	Pass	Pass	94
Picoxystrobin	0.998	0.5	6.53	-0.352	3.62	5.02	Pass	Pass	84
Piperonyl-butoxide	0.998	1.0	7.93	-0.817	13.43	12.84	Pass	Pass	88
Piperophos	0.999	0.5	7.37	-0.229	2.79	3.27	Pass	Pass	94
Pirimicarb	0.996	0.5	3.90	0.078	7.17	7.93	Pass	Pass	98
Pirimiphos-ethyl	0.999	0.5	7.82	-0.525	3.38	4.07	Pass	Pass	96
Pirimiphos-methyl	0.984	0.5	6.99	-0.111	3.11	4.33	Pass	Pass	100
Pretilachlor	0.998	0.5	7.51	0.604	6.06	4.62	Pass	Pass	98
Prochloraz	0.999	0.5	7.07	-0.579	3.88	3.83	Pass	Pass	100
Profenofos	0.997	0.5	7.74	0.146	6.76	4.19	Pass	Pass	95
Prometon	0.985	0.5	4.57	-0.048	11.59	6.19	Pass	Pass	100
Propachlor	0.996	0.5	4.94	0.043	3.94	4.44	Pass	Pass	100
Propamocarb	0.998	0.5	2.87	-0.756	4.83	5.16	Pass	Pass	98
Propaquizafop	0.999	0.5	7.85	-0.939	5.29	4.83	Pass	Pass	97
Propargite	0.999	0.5	8.29	-0.288	3.87	3.64	Pass	Pass	89
Propazine	0.999	0.5	5.51	0.262	1.92	1.95	Pass	Pass	100
Propetamphos	0.998	10.0	5.94	0.130	4.26	4.4	Pass	Pass	90
Propiconazole	0.998	0.5	6.99	-1.080	4.53	6.81	Pass	Pass	98
Propoxur	0.998	10.0	4.12	-0.061	3.87	3.71	Pass	Pass	98
Propyzamide	0.999	0.5	5.87	0.607	3.63	3.26	Pass	Pass	95
Prosulfocarb	0.999	0.5	7.59	0.616	2.15	2.01	Pass	Pass	100
Prothioconazole	0.998	10.0	6.95	-1.289	4.39	4.27	Pass	Pass	85
Pymetrozine	0.999	0.5	2.84	-1.480	7.8	9.1	Pass	Pass	91
Pyracarbolid	0.997	0.5	4.34	-0.099	5.87	5.21	Pass	Pass	95
Pyraclifos	0.999	0.5	7.13	0.284	5.04	4.35	Pass	Pass	96
Pyraclostrobin	0.999	0.5	7.07	-0.065	4.4	4.4	Pass	Pass	97
Pyrazophos	0.998	0.5	7.17	0.446	3.82	3.33	Pass	Pass	94
Pyrazosulfuron ethyl	0.999	0.5	6.16	0.117	4.8	4.61	Pass	Pass	89
Pyrazoxyfen	0.998	0.5	6.83	-1.904	6.38	4.65	Pass	Pass	91
Pyributicarb	0.999	0.5	8.04	0.772	3.14	3	Pass	Pass	97
Pyridaben	1.000	0.5	8.84	-0.314	4.7	4.68	Pass	Pass	98

Table 2. Name of compound, r², concentration LOQ, RT, Δppm, %RSD, FI, and Library Score

Compound	R ²	LOQ conc. (ppb)	Actual RT (min)	Δ m/z (ppm)	%RSD	% CV	LS	FI	Library score (%)
Pyridaphenthion	0.999	0.5	6.01	-0.387	2.59	2.43	Pass	Pass	96
Pyridate	0.999	1.0	9.23	-0.495	4.83	6.63	Pass	Pass	94
Pyrifenox	0.998	0.5	6.17	-0.078	11.62	18.29	Pass	Pass	96
Pyriftalid	0.999	0.5	5.43	-0.552	3.21	3.43	Pass	Pass	93
Pyrimethanil	0.999	0.5	5.74	0.026	3.12	3.96	Pass	Pass	100
Pyrimidifen	0.999	0.5	8.03	0.148	1.18	1.38	Pass	Pass	98
Pyriproxyfen	0.999	0.5	8.10	-0.289	2.35	2.33	Pass	Pass	96
Pyroquilon	0.951	0.5	4.45	-0.268	4.48	5.12	Pass	Pass	94
Pyroxsulam	0.998	0.5	4.11	0.223	4.25	4.01	Pass	Pass	82
Quinalphos	1.000	0.5	6.76	-0.337	2.25	2.11	Pass	Pass	90
Quinoclamine	0.919	1.0	4.23	-0.313	10.58	6.12	Pass	Pass	92
Quinoxifen	0.999	0.5	8.48	-0.108	3.98	4.51	Pass	Pass	92
Rabenzazole	0.996	0.5	5.01	-0.241	6.72	5.84	Pass	Pass	90
Resmethrin	0.999	0.5	8.98	-0.194	4.85	4.62	Pass	Pass	78
Rotenone	0.998	0.5	6.46	-0.501	3.59	2.95	Pass	Pass	95
Saflufenacil	0.997	10.0	5.23	0.176	5.96	5.65	Pass	Pass	84
Schradan	0.997	0.5	3.48	0.242	7.51	7.14	Pass	Pass	88
Sebuthylazine	0.999	0.5	5.51	0.262	1.92	1.95	Pass	Pass	95
Secbumeton	0.983	0.5	4.57	-0.048	10.04	6.19	Pass	Pass	100
Sethoxydim	0.999	0.5	7.80	-0.181	5.99	5.77	Pass	Pass	83
Siduron	0.998	0.5	5.57	-1.240	5.59	4.68	Pass	Pass	97
Simeconazole	0.998	0.5	6.23	0.136	6.42	4.9	Pass	Pass	92
Simetryn	0.999	0.5	4.44	-0.066	4.06	4.17	Pass	Pass	86
Spinetoram 1	0.998	0.5	7.46	-2.242	4.47	5.14	Pass	Pass	86
Spirodiclofen	0.999	0.5	8.54	0.116	4.46	4.63	Pass	Pass	96
Spiroxamine	0.999	0.5	5.65	0.369	7.2	7.03	Pass	Pass	99
Sulcotrione	0.991	100.0	3.85	-1.374	12.84	13.25	Pass	Pass	100
Sulfallate	0.998	10.0	6.84	-0.486	7.42	8.14	Pass	Pass	90
Sulfentrazone	0.998	10.0	4.25	-0.589	7.83	5.19	Pass	Pass	92
Sulfotep	0.999	0.5	6.73	-0.224	4.63	5.62	Pass	Pass	91
Sulprofos	0.999	0.5	8.29	-0.263	10.57	7.61	Pass	Pass	84
Tebuconazole	0.997	0.5	6.78	0.050	14.74	4.34	Pass	Pass	100
Tebupirimfos	0.999	0.5	7.88	-0.055	5.43	6.21	Pass	Pass	92
Tebutam	0.999	0.5	6.36	0.138	2.04	2.2	Pass	Pass	99
Tebuthiuron	0.999	0.5	4.30	1.578	7.39	7.33	Pass	Pass	92
Temephos	0.999	10.0	7.99	-0.568	5.85	5.93	Pass	Pass	90
TEPP	0.997	0.5	3.85	0.992	11.4	12.47	Pass	Pass	76
Tepraloxydim	0.998	0.5	6.15	0.468	5.76	4.25	Pass	Pass	82
Terbucarb	1.000	0.5	7.37	-1.768	7.57	7.63	Pass	Pass	99
Terbufos	0.998	10.0	7.85	3.632	11.12	11.83	Pass	Pass	87
Terbufos_M-C4H7	0.997	10.0	7.85	0.590	6.56	6.83	Pass	Pass	84
Terbufos-sulfone	0.999	0.5	5.39	0.188	7.66	8.78	Pass	Pass	81
Terbumeton	0.990	1.0	4.57	0.492	4.85	3.02	Pass	Pass	100
Terbuthylazine	0.997	0.5	5.70	-0.070	3.35	3.03	Pass	Pass	100

Table 2. Name of compound, r², concentration LOQ, RT, Δppm, %RSD, FI, and Library Score

Compound	R ²	LOQ conc. (ppb)	Actual RT (min)	Δ m/z (ppm)	%RSD	% CV	LS	FI	Library score (%)
Terbutryn	0.997	1.0	5.79	0.176	2.87	2.94	Pass	Pass	100
Tetrachlorvinphos	0.999	0.5	6.56	-0.015	4.94	4.48	Pass	Pass	91
Tetraconazole	0.998	0.5	6.28	-0.168	8.89	6.81	Pass	Pass	93
Tetramethrin	0.997	0.5	7.76	0.117	6.07	4.34	Pass	Pass	91
Thenylchlor	0.999	0.5	6.22	-0.503	3.81	4.4	Pass	Pass	86
Thiabendazole	0.999	0.5	3.45	-0.101	7.15	7.59	Pass	Pass	96
Thiacloprid	0.999	0.5	3.63	0.762	8.4	7.76	Pass	Pass	93
Thiazopyr	0.999	0.5	6.71	0.313	4.9	5.51	Pass	Pass	99
Thifensulfuron-methyl	0.999	0.5	4.05	-0.958	11.81	12.08	Pass	Pass	87
Thiobencarb	0.999	10.0	7.15	0.318	3.7	3.77	Pass	Pass	86
Thiodicarb	0.999	0.5	4.64	-1.075	5.18	5.57	Pass	Pass	83
Thiofanox sulfoxide	0.999	10.0	3.27	-0.155	3.38	3.38	Pass	Pass	86
Thiophanate-methyl	0.998	0.5	4.07	1.327	5.97	6.04	Pass	Pass	84
Tolyfluanid	0.997	10.0	6.71	-0.177	5.4	5.46	Pass	Pass	93
Triadimefon	0.999	0.5	5.89	0.597	2.67	2.45	Pass	Pass	88
Triadimenol	0.997	1.0	6.09	-0.317	3.62	3.44	Pass	Pass	95
Triallate	0.996	10.0	8.22	0.014	6.01	6.89	Pass	Pass	86
Triazamate	0.999	0.5	6.06	0.062	3.25	3.81	Pass	Pass	87
Triazophos	0.998	0.5	6.12	0.246	3.26	3.44	Pass	Pass	94
Tributyl phosphate	0.999	1.0	7.49	0.216	4.17	2.49	Pass	Pass	89
Tricyclazole	0.999	0.5	3.98	0.375	7.55	8.02	Pass	Pass	95
Trietazine	0.998	0.5	6.25	0.063	3.97	4.97	Pass	Pass	100
Trifloxystrobin	0.999	0.5	7.37	-0.316	4.79	4.55	Pass	Pass	96
Triflumizole	0.999	0.5	7.62	-0.221	2.96	3.76	Pass	Pass	93
Triflumuron	0.991	0.5	7.13	0.132	9.29	3.75	Pass	Pass	98
Tri-Isobutyl phosphate	0.999	1.0	7.49	0.216	4.11	2.49	Pass	Pass	92
Trinexapac-ethyl	0.993	10.0	5.08	-0.460	8.6	8.43	Pass	Pass	99
Uniconazole	0.996	0.5	6.50	0.641	4.95	2.86	Pass	Pass	92
Vamidotion	0.998	0.5	3.37	0.131	2.4	2.39	Pass	Pass	86
Vernolate	0.999	0.5	7.27	0.536	6.46	7.28	Pass	Pass	92
Warfarin	0.996	0.5	5.66	0.039	6.52	4.24	Pass	Pass	97
Zinophos	0.999	0.5	4.96	-0.181	8.93	9.84	Pass	Pass	86
Zoxamide	0.998	0.5	6.91	-0.146	8.04	5.92	Pass	Pass	83

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