

Confirmation of Pesticides in Jalapeno Peppers Using QTRAP[®] MS/MS Data and Library Matching in SCIEX OS-Q

Combining Enhanced Product Ion Scan with the Latest Software for High Confidence Confirmation

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What: Food testing labs are frequently confronted with the need for more confirmatory information when it comes to analyte identification in real-world samples. In complex matrices, interferences may complicate interpretation of data resulting in false positives or reported residue levels to come into question. Combining QTRAP[®] technology with the latest software tools of SCIEX OS-Q allows for the collection of full-scan MS/MS spectra for targeted pesticides in complex food samples. Those MS/MS data can be subsequently searched against SCIEX verified libraries for unambiguous qualitative confirmation of pesticide detection and ID.

How: The MS method was set up with a targeted MRM list of 200+ pesticides. IDA (Information Dependent Acquisition) criteria were defined such that Enhanced Product Ion (EPI) acquisition would be triggered when an MRM signal exceeded a threshold of 2000 cps. This type of data acquisition results in the collection of MS/MS spectral information in addition to the MRM signal (Fig. 1). Samples of dried, canned, and fresh jalapeno peppers were extracted and analyzed for the

pesticide panel. Data were processed in SCIEX OS-Q for quantitation by MRM and spectral identification by library matching. Figure 2 shows collected MS/MS spectra being used to confirm the identity of the MRM peak in the pepper extract. This additional stringency in identity confirmation could help protect against reporting false positive detections for residues in complex samples.

Sample Name	Sample	Component	Actual Conc.	Reported RT	Area	Retention Time	Retention Time Error	Signal	Library Conf.	Library Name	Library RT
JKU-C	Unknown	Chlorantraniliprole	N/A	5.40	3.88E+04	5.53	2.339	14.6	✓	Chlorantraniliprole	75.4
JKU-C	Unknown	Difenoconazole	N/A	4.70	1.89E+04	4.40	6.487	388.5	✓	Difenoconazole	88.9
JKU-C	Unknown	Difenoconazole	N/A	13.32	1.53E+04	13.17	3.063	473.0	✓	Difenoconazole	88.9
JKU-C	Unknown	Imidacloprid	N/A	4.77	1.87E+04	4.74	4.844	713.0	✓	Imidacloprid	88.9
JKU-C	Unknown	Thiamethoxam	N/A	6.00	2.20E+04	6.33	1.233	2348.0	✓	Thiamethoxam (MS)	88.7
JKU-C	Unknown	Thiamethoxam	N/A	3.27	4.43E+04	3.32	7.762	282.2	✓	Thiamethoxam	88.9
JKU-C	Unknown	αB-Albacore	1.00	9.19	7.01E+04	9.30	0.955	282.8	✓	Albacore αB (Direct)	88.0
JKU-C	Unknown	Asopropalin	N/A	10.90	1.13E+04	10.96	0.564	59.2	✓	Asopropalin (MS)	83.2
JKU-C	Unknown	Chlorantraniliprole	N/A	5.40	1.52E+04	5.42	0.077	31.8	✓	Chlorantraniliprole	88.8
JKU-C	Unknown	Difenoconazole	N/A	4.70	8.83E+04	4.30	4.434	128.9	✓	Difenoconazole	88.0
JKU-C	Unknown	Difenoconazole	N/A	13.32	1.07E+04	13.18	1.199	958.8	✓	Difenoconazole (MS)	88.6
JKU-C	Unknown	Imidacloprid	N/A	4.77	4.81E+04	4.48	6.330	242.9	✓	Imidacloprid	88.9
JKU-C	Unknown	Thiamethoxam	N/A	6.00	1.54E+04	6.29	4.239	653.5	✓	Thiamethoxam	108.0
JKU-C	Unknown	Thiamethoxam	N/A	3.27	2.08E+04	3.88	6.993	265.1	✓	Thiamethoxam	88.2
JKU-C	Unknown	αB-Albacore	1.00	9.19	6.77E+04	9.30	1.443	333.0	✓	Albacore αB (Direct)	88.0
CDU-B	Unknown	Ethioniazole	N/A	12.84	4.23E+04	12.85	0.208	11.9	✓	α-Hydroxyethioniazole	72.7
CDU-B	Unknown	αB-Albacore	1.00	9.19	4.01E+04	9.85	6.675	188.2	✓	α-Hydroxyethioniazole	83.2
CDU-B	Unknown	αB-Albacore	1.00	10.15	9.47E+04	10.04	1.993	31.1	✓	1-Propylthio-αB-Albacore	87.6

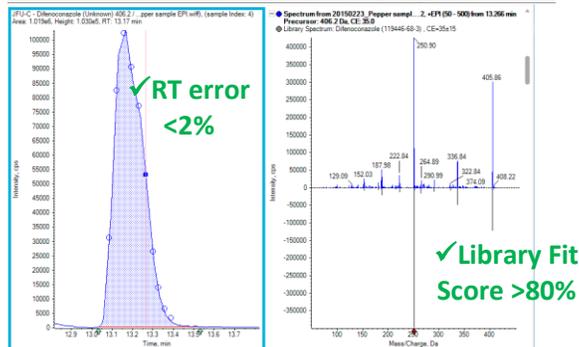


Figure 2. High confidence in positive detection possible with QTRAP and SCIEX OS-Q. ID and quantitation of pesticides can be achieved with high confidence using QTRAP to collect MS/MS spectra in addition to MRM peaks. Retention time and MS/MS pattern are compelling evidence that the identified peak is Difenoconazole. Circles on the chromatographic peak represent where EPI scan has been triggered; the software automatically chooses which spectrum is the highest quality and displays it on the right. The colored circle denotes which scan is being displayed. SCIEX OS-Q results table quickly shows with green check marks in the Confidence columns where peaks have been confirmed with RT error <2% and library fit score of >80%. Rapid visual assessment of large sample sets is possible, ultimately resulting in greater efficiency and increased qualitative confidence in reported detects during data processing for residues in food samples.

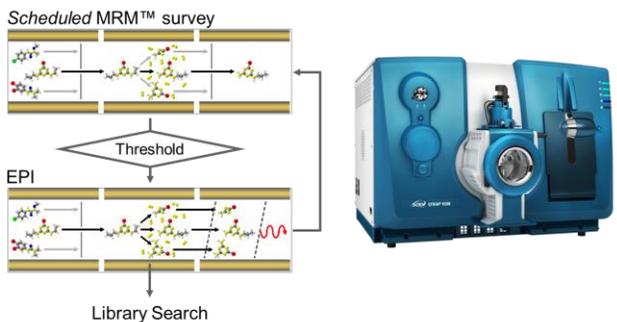


Figure 1. The QTRAP[®] 4500 system was employed with EPI scan type triggered by signal from target pesticides monitored in MRM mode. The resulting MS/MS spectrum were matched to library spectra for confirmation.

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