Application Note

Cannabis & Hemp Testing

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Automated MRM Method Development for Pesticides in Cannabis Using the Agilent MassHunter Optimizer for GC/TQ

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Abstract

This application note demonstrates the use of Agilent MassHunter Optimizer for GC/TQ to enable highly automated, end-to-end development of multiple reaction monitoring (MRM) data acquisition methods. The Optimizer for GC/TQ uses spectral deconvolution to reliably identify precursor ions, even in the presence of chromatographic interferences. This tool enables significant time savings and reduces manual review when developing MRM data acquisition methods. A mix of 25 cannabis-related pesticides regulated in California and Canada was used to test the process.

Key advantages of the Optimizer tool include:

- Time-savings for developing an optimized MRM method
- Automation and reduced manual work
- Reproducibility
- A smooth transition of GC/MSD methods to GC/TQ
- Built-in review tools

Introduction

Development of GC/MS/MS MRM transitions is a challenging and time-consuming multistep process, which may be further complicated by analyte coelution and matrix interferences. This has traditionally required manual intervention by an experienced scientist. MassHunter Optimizer for GC/TQ enables automated optimization of the data acquisition parameters for MRM mode.

End-to-end MRM method development can be highly automated, with no user interaction. Alternatively, each of the optimization steps can be performed individually. These steps include:

- Identification of the analytes using library search of deconvoluted spectra
- Precursor ion identification
- Product ion identification at various collision energies
- Selection of product ions
- Optimization of collision energy

Several workflows available with the Optimizer for GC/TQ, such as *Start from scan data* and *Start from SIM ions*, allow new GC/TQ users to convert existing single quadrupole scan or SIM methods to triple quadrupole MRM methods. Existing TQ users can re-optimize collision energies for current MRMs and update their retention times under new chromatographic conditions with the *Start with MRMs* workflow.

In this work, an MRM acquisition method was developed for 25 GC-amenable pesticides regulated in cannabis in California by the Bureau of Cannabis Control (BCC)[1] and in Canada by Health Canada.[2] These compounds commonly stand out as challenging to analyze using electrospray LC/MS.

Up to 18 MRM transitions were developed for each compound using a pesticide standard mixture in solvent following the *Start from scan data* workflow. Then, the collision energies for the developed MRM transitions were re-optimized in cannabis matrix. The final, matrix-optimized MRM acquisition method included up to five transitions per compound and enabled the highest selectivity for target pesticides in a challenging cannabis matrix.

Experimental

MassHunter Optimizer for GC/TQ is installed automatically with Agilent MassHunter GC/MS Data Acquisition Version 10.0 and above. It is supported for use with Agilent 7000 series and 7010 series GC/TQ. A desktop icon is created when a GC/MS instrument is configured using the Agilent GC/MS configuration tool. To start MRM development, an existing data acquisition method is required. All GC parameters of the acquisition method will be retained when developing and optimizing MRM transitions.

The software offers several workflows that can be used when developing and optimizing MRM transitions. Choice of workflow depends on the starting acquisition method. These workflows include:

- *Start from scan data*
- *Start from SIM ions*
- *Start from MRMs*

This application note describes the *Start from scan data* workflow, covering the entire MRM development process. An Agilent 8890/7010B GC/TQ system and Agilent MassHunter workstation revision 10, including MassHunter acquisition 10 SR1, were used in this work. The starting acquisition method was previously optimized for successful GC analysis of pesticides in cannabis.[3] In the *Start from scan data* workflow, the mass spectrometer was operated in full scan mode (MS2) to acquire the scan data file for compound identification and precursor ion selection, performing the scan over an *m/z* 35 to 450 range with a scan time of 140 ms.

The *Start from scan data* workflow includes the following steps performed sequentially:

- Acquisition or import of full scan data to identify target compounds
- Precursor ion identification
- Product ion identification
- Collision energy optimization

When starting from scan, the first step of MRM development is identification of the analytes using a library search of deconvoluted spectra. This allows correct identification of target analytes and enables reliable selection of precursor ions, even in the presence of chromatographic interferences such as column bleed, coeluting analytes, or matrix interference. The spectral deconvolution and library search algorithms are similar to what is used with Agilent MassHunter Unknowns Analysis software. Library formats supported by the Optimizer for GC/TQ include *.L and *.mslibrary.xml. This provides the flexibility of using large spectral libraries such as NIST or small user-created libraries built with Agilent MassHunter library editor software. In this application note, a user-made pesticide library that included only the target compounds was used.

The latter three steps in MRM development can be highly automated, with no user intervention. Alternatively, the result of each step can be reviewed before proceeding to the next step. Before proceeding, the user may modify automated selections and select additional ions if desired. In this application note, precursors selected for target pesticides were reviewed before proceeding to the following optimization steps. The rest of the MRM optimization presented here was fully automated.

After MRM development and collision energy optimization are complete, the developed acquisition method can be saved as a time-segment MRM method or a dynamic MRM (dMRM) method. The latter option allows the user to define minimum dwell time and number of cycles per second.

It is recommended to perform initial MRM development using a neat solvent standard containing the compounds of interest at a concentration easily detectable with a GC/TQ system. Collision energies for the developed transitions can be re-optimized in matrix, as shown in this application note.

Results and discussion

Library search and precursor ion identification

Twenty-five pesticides were identified using an acquired full scan chromatogram of a standard mixture by searching deconvoluted mass spectra against a custom-built pesticide library. Figure 1A demonstrates the Optimizer window after completing compound identification. It includes:

- A compound table.
- A chromatogram with labeled peaks.
- A deconvoluted mass spectrum.
- Precursor ions available for each compound.
- A summary of all precursor ions selected for all identified compounds. A complete compound table is shown in Figure 1B.

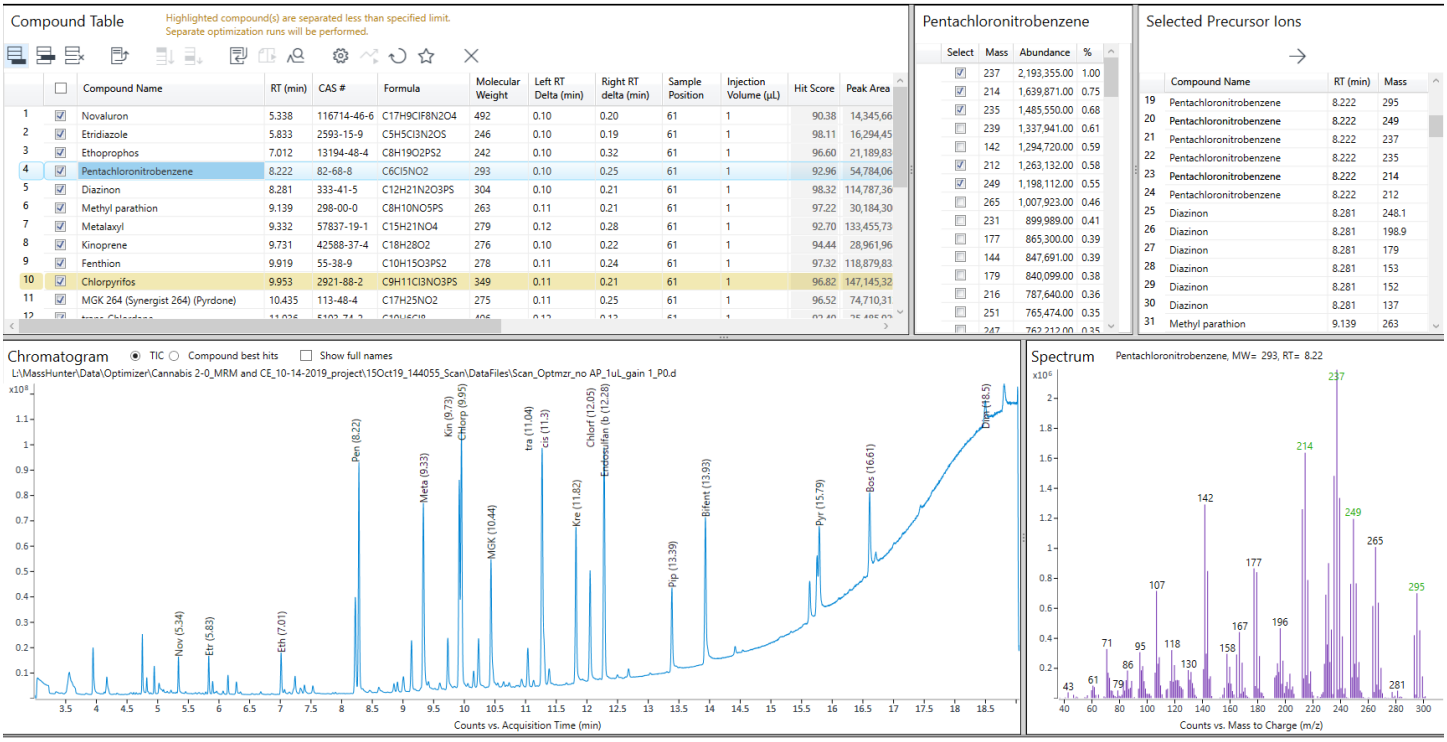
A library match score is displayed in the table in Figure 1 under the Hit Score column. Information available in the library such as compound name, CAS number, molecular formula, and molecular weight is imported into the Compound Table in the Optimizer. A deconvoluted spectrum for each identified compound is displayed when selecting it in the compound table. Figure 2 demonstrates a deconvoluted spectrum for pentachloronitrobenzene (also known as quintozene) with the suggested precursor ions highlighted in green. Spectral deconvolution enables correct compound identification and reliable choice of precursor ions, even in the presence of chromatographic interferences such as column bleed or a coeluting peak.

The list of available precursor ions is displayed when selecting a corresponding compound in the compound table. Figure 3A demonstrates a portion of precursor ions available for pentachloronitrobenzene. The ions selected in the table were chosen as precursor ions automatically by the software, as the Optimizer method was set up to pick no more than six ions as precursors for each compound (Figure 3B).

Note the choice of precursors suggested by the software is based on the abundance and *m/z* value. Also, no more than two ions from a cluster are selected. For example, a molecular ion for pentachloronitrobenzene, *m/z* 295, was automatically selected as a precursor ion because of its high *m/z* value and uniqueness, despite not being among the most abundant ion in the spectrum. Precursors suggested by the software can be overwritten by the user by unchecking selected ions and checking available ones.

The following MRM development steps (i.e., product ion identification and collision energy optimization) can be automated, requiring the user to review only the final optimized transitions. It can also be done step by step in sequence, allowing the user to review the selection of product ions before performing the collision energy optimization step.

A



B

Compound Table

Highlighted compound(s) are separated less than specified limit.
Separate optimization runs will be performed.

	Compound Name	RT (min)	CAS #	Formula	Molecular Weight	Left RT Delta (min)	Right RT delta (min)	Sample Position	Injection Volume (µL)	Hit Score	Peak Area	Data f
1	Novaluron	5.338	116714-46-6	C17H9ClF8N2O4	492	0.10	0.20	61	1	90.38	14,345,663.00	L:\Mas
2	Etridiazole	5.833	2593-15-9	C5H5Cl3N2OS	246	0.10	0.19	61	1	98.11	16,294,451.00	L:\Mas
3	Ethoprophos	7.012	13194-48-4	C8H19O2PS2	242	0.10	0.32	61	1	96.60	21,189,836.00	L:\Mas
4	Pentachloronitrobenzene	8.222	82-68-8	C6Cl5NO2	293	0.10	0.25	61	1	92.96	54,784,068.00	L:\Mas
5	Diazinon	8.281	333-41-5	C12H21N2O3PS	304	0.10	0.21	61	1	98.32	114,787,360.00	L:\Mas
6	Methyl parathion	9.139	298-00-0	C8H10NO5PS	263	0.11	0.21	61	1	97.22	30,184,300.00	L:\Mas
7	Metalaxyl	9.332	57837-19-1	C15H21NO4	279	0.12	0.28	61	1	92.70	133,455,736.00	L:\Mas
8	Kinoprene	9.731	42588-37-4	C18H28O2	276	0.10	0.22	61	1	94.44	28,961,968.00	L:\Mas
9	Fenthion	9.919	55-38-9	C10H15O3PS2	278	0.11	0.24	61	1	97.32	118,879,832.00	L:\Mas
10	Chlorpyrifos	9.953	2921-88-2	C9H11Cl3NO3PS	349	0.11	0.21	61	1	96.82	147,145,328.00	L:\Mas
11	MGK 264 (Synergist 264) (Pyrdone)	10.435	113-48-4	C17H25NO2	275	0.11	0.25	61	1	96.52	74,710,312.00	L:\Mas
12	trans-Chlordane	11.036	5103-74-2	C10H6Cl8	406	0.12	0.13	61	1	92.40	25,485,920.00	L:\Mas
13	Endosulfan (alpha isomer)	11.269	959-98-8	C9H6Cl6O3S	404	0.13	0.25	61	1	98.52	172,941,552.00	L:\Mas
14	cis-Chlordane	11.299	5103-71-9	C10H6Cl8	406	0.18	0.16	61	1	79.24	11,491,115.00	L:\Mas
15	Kresoxim-methyl	11.821	143390-89-0	C18H19NO4	313	0.11	0.25	61	1	96.33	91,899,800.00	L:\Mas
16	Chlorfenapyr	12.051	122453-73-0	C15H11BrClF3N2O	406	0.11	0.14	61	1	97.62	65,994,096.00	L:\Mas
17	Endosulfan (beta isomer)	12.280	33213-65-9	C9H6Cl6O3S	404	0.12	0.27	61	1	98.34	155,355,504.00	L:\Mas
18	Piperonyl butoxide	13.386	51-03-6	C19H30O5	338	0.12	0.24	61	1	96.50	49,822,004.00	L:\Mas
19	Bifenthrin	13.931	82657-04-3	C23H22ClF3O2	422	0.12	0.25	61	1	94.68	91,573,560.00	L:\Mas
20	Bifenazate	13.964	149877-41-8	C17H20N2O3	300	0.21	0.26	61	1	58.53	4,678,718.00	L:\Mas
21	(1R)-cis-Permethrin	15.632	54774-46-8	C21H20Cl2O3	390	0.12	0.19	61	1	90.74	25,467,686.00	L:\Mas
22	(1R)-trans-Permethrin	15.751	61949-77-7	C21H20Cl2O3	390	0.11	0.24	61	1	94.19	35,526,228.00	L:\Mas
23	Pyridaben	15.787	96489-71-3	C19H25ClN2OS	364	0.11	0.21	61	1	93.84	51,883,384.00	L:\Mas
24	Boscalid (Nicobifen)	16.610	188425-85-6	C18H12Cl2N2O	342	0.13	0.23	61	1	80.58	51,811,116.00	L:\Mas
25	Dimethomorph-(Z) {CAS # 110488-70-5}	18.495	999012-03-2	C21H22ClNO4	387	0.15	0.22	61	1	80.00	17,733,326.00	L:\Mas

Figure 1. The Agilent MassHunter Optimizer for GC/TQ window displaying compound identification results (A) and a zoomed-in compound table with 25 pesticides identified in a full scan chromatogram using mass spectrum deconvolution with a library search. Compounds that coelute are highlighted in yellow. These compounds were optimized by separate injections (B).

A

Pentachloronitrobenzene

Select	Mass	Abundance	%
☑	237	2,193,355.00	1.00
☑	214	1,639,871.00	0.75
☑	235	1,485,550.00	0.68
☐	239	1,337,941.00	0.61
☐	142	1,294,720.00	0.59
☑	212	1,263,132.00	0.58
☑	249	1,198,112.00	0.55
☐	265	1,007,923.00	0.46
☐	231	899,989.00	0.41
☐	177	865,300.00	0.39
☐	144	847,691.00	0.39
☐	179	840,099.00	0.38
☐	216	787,640.00	0.36
☐	251	765,474.00	0.35
☐	247	762,212.00	0.35
☐	107	715,275.00	0.33
☑	295	700,222.00	0.32
☐	229	690,256.00	0.31
☐	267	637,114.00	0.29
☐	263	614,898.00	0.28
☐	196	466,621.00	0.21
☐	233	457,829.00	0.21
☐	297	452,516.00	0.21
☐	167	441,127.00	0.20
☐	293	419,980.00	0.19
☐	241	411,835.00	0.19
☐	230	358,725.00	0.16
☐	71	327,703.00	0.15
☐	118	320,587.00	0.15
☐	95	306,603.00	0.14
☐	143	297,288.00	0.14
☐	158	295,652.00	0.13
☐	165	291,360.00	0.13
☐	181	281,125.00	0.13
☐	109	272,908.00	0.12
☐	198	250,281.00	0.11
☐	253	241,333.00	0.11
☐	232	241,168.00	0.11

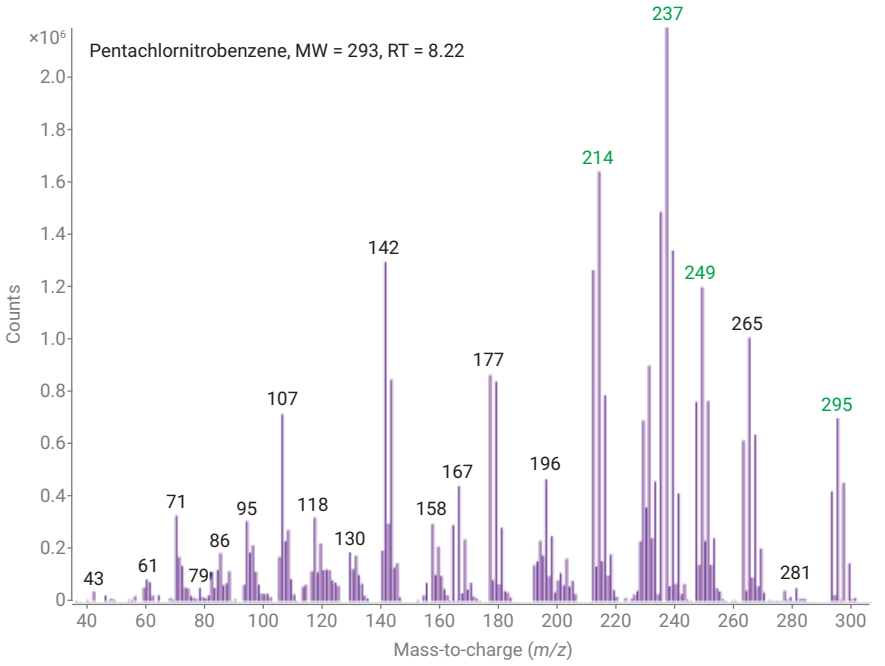


Figure 2. Deconvoluted mass spectrum of pentachloronitrobenzene with suggested precursor ions highlighted in green.

B

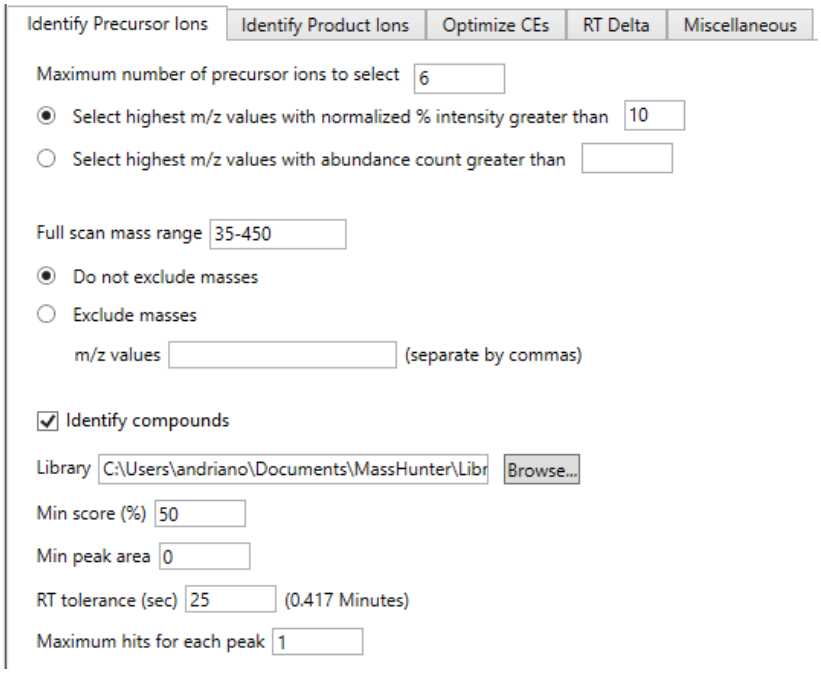


Figure 3. Precursor ions suggested for pentachloronitrobenzene (A) and precursor identification parameters (B).

Product ion identification

Product ion identification for each precursor ion is performed via a product ion scan at multiple collision energies defined by the user. Maximum four collision energies are permitted for product ion scan. In this work, product ion scan experiments were performed at default values of 5, 15, 25, and 35 eV. Product ion optimization may require several injections depending on the number of precursor ions per analyte and how well the targets are chromatographically resolved. It is recommended to have the analytes chromatographically baseline-resolved to ensure the most effective MRM development. However, MRM development can be performed for coeluting compounds if their mass spectra differ and the compound response abundance is comparable. To perform MRM development for coeluting targets, additional injections may be needed. In this work, several pesticides in the standard coeluted as indicated by yellow highlighting in the compound table in Figure 1B. It took 12 injections to obtain the product ion scans for all the target pesticides: six injections for each of the six precursor ions per compound, and another six injections for the highlighted coeluting compounds.

Product ion identification results are shown in Figure 4A, with pentachloronitrobenzene highlighted in the product ion scan table. The window includes:

- A product ion scan table, in which each line corresponds to one precursor ion
- A total ion chromatogram (TIC) or extracted ion chromatograms (EIC) for each of the precursors acquired at four different collision energies
- Product ion scan mass spectra for the highlighted precursor acquired at four different collision energies
- A table with product ions available for the highlighted precursor
- A summary of all product ions selected.

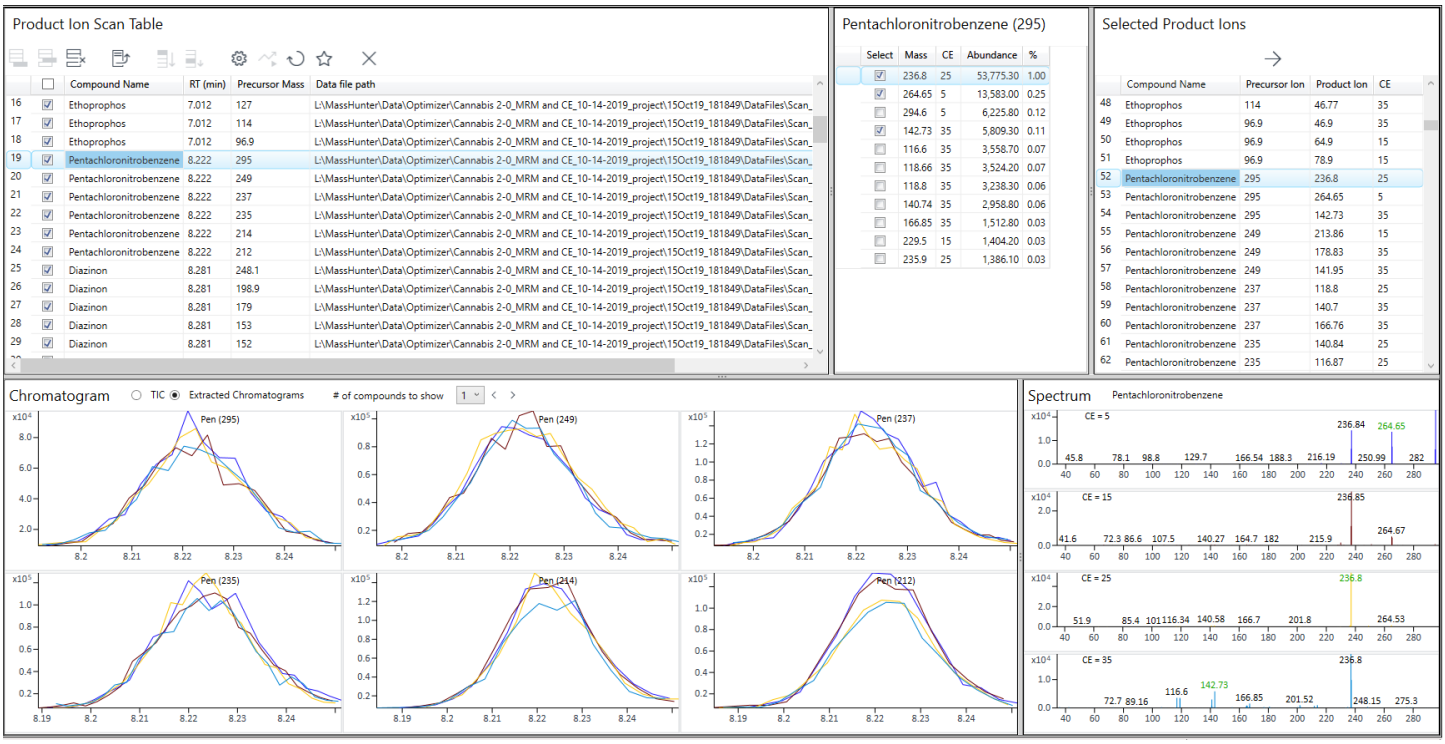
Product ion identification parameters are shown in Figure 4B. Selection of product ions is based on their abundance, as shown for the precursor (*m/z* 295) for pentachloronitrobenzene in Figure 4A. If a manual revision of the product ion identification step is performed, product ions suggested by the software can be overwritten by the user by unchecking selected ions and checking available ones.

Collision energy optimization

Collision energy optimization can be performed around the value chosen in the previous step or over a defined range. In this work, collision energies were optimized for 375 MRM transitions over a range of 0 to 60 eV with a step size of 5 eV (Figure 5B) by performing six injections. This step would require only three injections instead of six if no coelution occurred or if coeluting compounds were ignored. Collision energy optimization results are shown in Figure 5A, with the 295 → 236.8 transition for pentachloronitrobenzene highlighted in the MRM transitions table. The window includes:

- An MRM transitions table, in which each line corresponds to one MRM transition
- TIC or EICs for each of the transitions acquired at all the tested collision energy values
- An ion breakdown profile, which demonstrates a plot of the MRM transition abundance versus collision energy
- Collision energies with corresponding abundances for the highlighted MRM transition

A



B

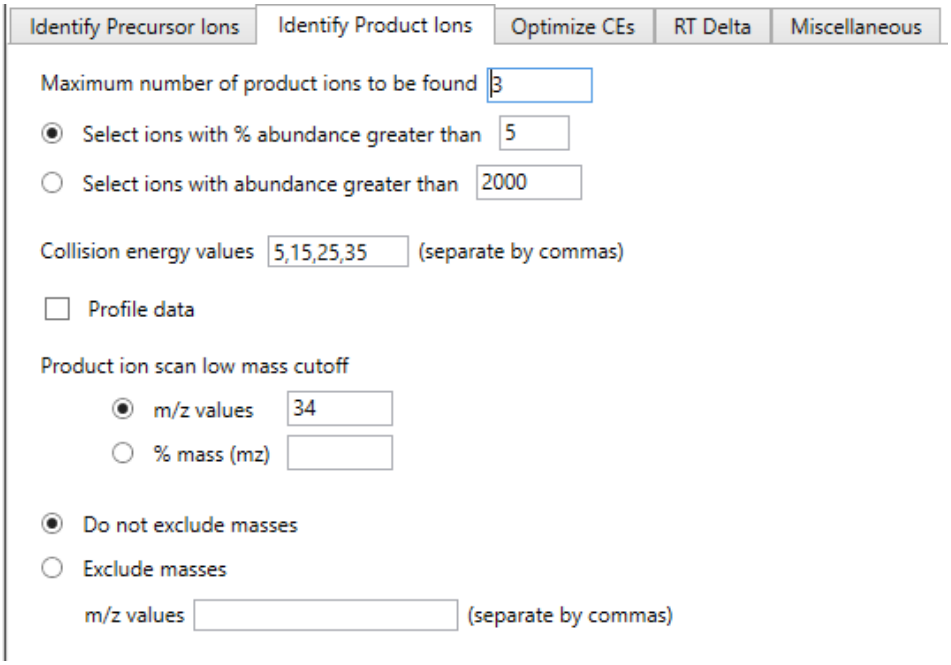
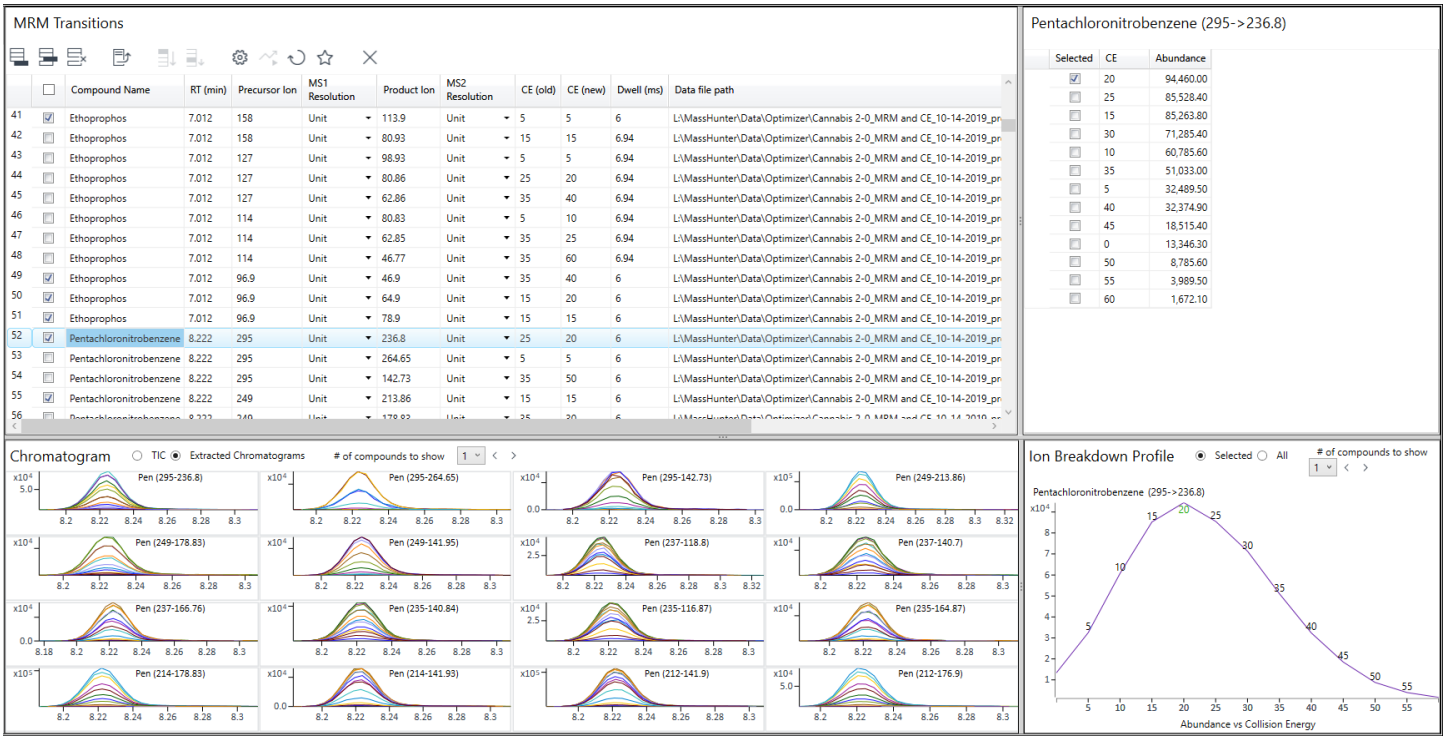


Figure 4. Product ion identification results with a precursor (*m/z* 295) for pentachloronitrobenzene highlighted in the product ion scan table (A) and product ion identification parameters (B).

A



B

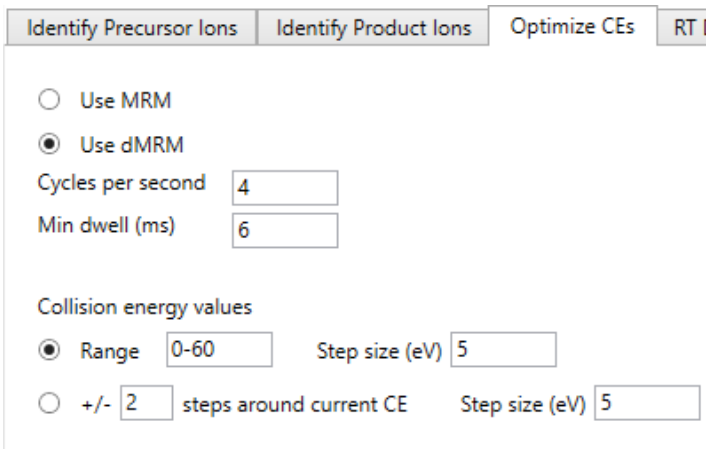


Figure 5. Collision energy optimization results with the 295 → 236.8 transition for pentachloronitrobenzene highlighted in the MRM transitions table (A) and collision energy optimization parameters (B).

Collision energy re-optimization in dried cannabis flower extract matrix

Re-optimizing collision energies in matrix is optional. Performing this step can help enhance the selectivity of the method. In this work, collision energies for the MRM transitions developed in solvent were re-optimized with dried cannabis flower extract matrix. For the majority of the target compounds, optimal collision energy in matrix appeared to be similar to the one optimized in solvent. Transition 165 → 121 for dimethomorph was shown to yield a higher response in cannabis matrix, with a higher collision energy compared to the value optimized in solvent (i.e., 20 eV versus 15 eV) (Figure 6). Furthermore, a higher collision energy of 25 eV can be used for dimethomorph in cannabis matrix with almost no loss in its response. In some matrices, a higher collision energy could yield a better signal-to-noise ratio.

The MRM transitions that did not have interferences from cannabis matrix were included in the final developed acquisition method, ensuring the best selectivity of the optimized MRM method.

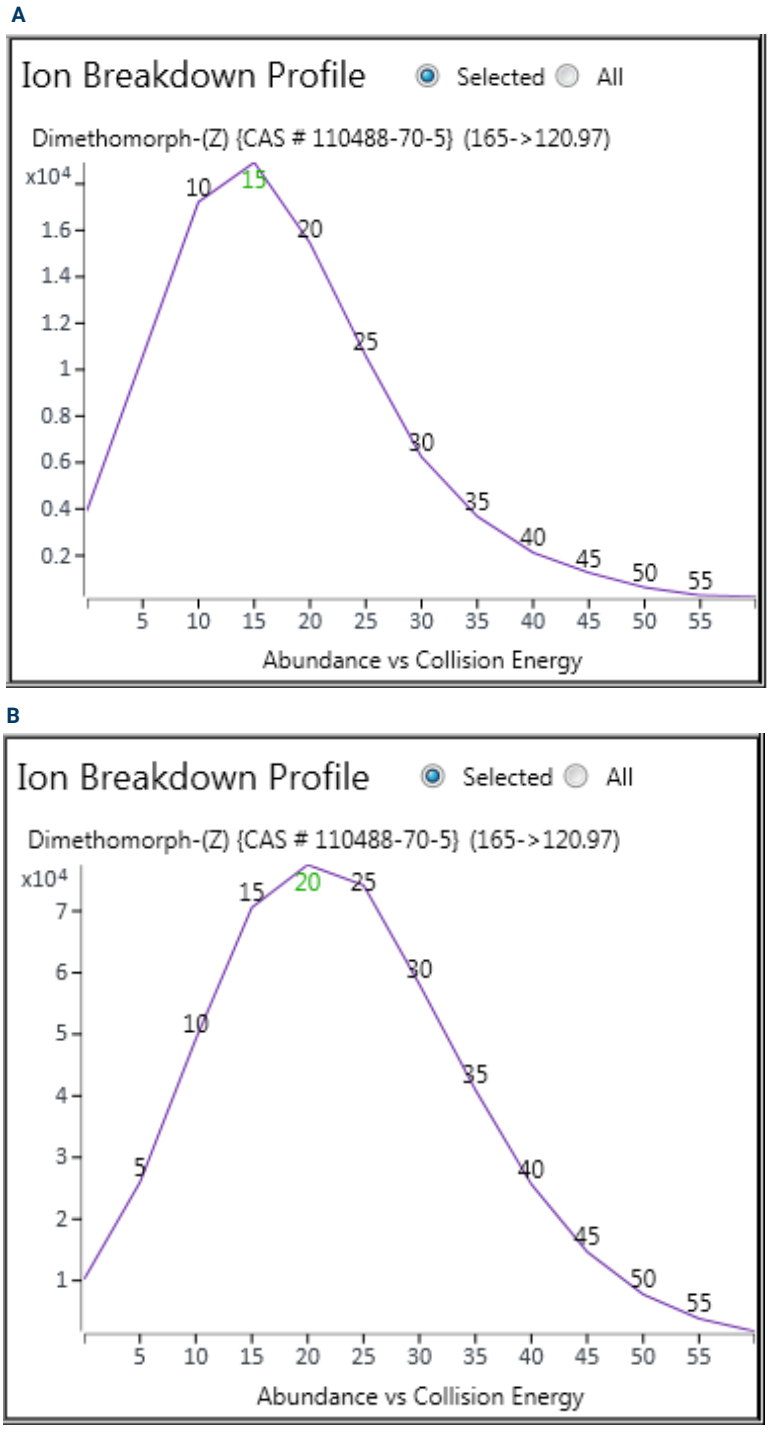


Figure 6. Ion breakdown profiles for the 165 → 121 MRM transition for dimethomorph in solvent (A) and in dried cannabis flower extract (B).

Reviewing results and saving method

When collision energy optimization is complete, the results are reviewed, and the acquisition method is saved. Information on all the developed transitions is available in the expanded table view under the Results (Figure 7A).

The number of top-ranked MRM transitions to be saved is defined by the number specified under *Select number of top ranked transitions*; only the checked MRM transitions will be included in the acquisition method. In this work, the five most abundant transitions that did not have interferences in cannabis matrix were selected.

To simplify method review, a nested view of the results table is available (Figure 7B), and its expanded view for pentachloronitrobenzene is shown in Figure 7C.

A

Optimized MRM Transitions — Select number of top ranked transitions: 5 — Left RT Delta (min): 0.20 — Right RT delta (min): 0.20 — Overwrite RT Delta — Nested View

		Compound Name	RT (min)	Precursor Ion	MS1 Resolution	Product Ion	MS2 Resolution	CE	Abundance	%	CAS #	Formula	Molecular Weight	Left RT Delta (min)	Right RT delta (min)	Sample Position	Injection Volume (µL)
52	☑	Pentachloronitrobenzene	8.222	249	Unit	213.86	Unit	15	136,955.33	1.00	82-68-8	C6Cl5NO2	293	0.10	0.25	61	1
53	☑	Pentachloronitrobenzene	8.222	212	Unit	141.9	Unit	40	112,122.61	0.82	82-68-8	C6Cl5NO2	293	0.10	0.25	61	1
54	☑	Pentachloronitrobenzene	8.222	214	Unit	178.83	Unit	15	107,271.52	0.78	82-68-8	C6Cl5NO2	293	0.10	0.25	61	1
55	☑	Pentachloronitrobenzene	8.222	212	Unit	176.9	Unit	15	94,933.50	0.69	82-68-8	C6Cl5NO2	293	0.10	0.25	61	1
56	☑	Pentachloronitrobenzene	8.222	295	Unit	236.8	Unit	20	94,459.98	0.69	82-68-8	C6Cl5NO2	293	0.10	0.25	61	1
57	☐	Pentachloronitrobenzene	8.222	249	Unit	141.95	Unit	60	71,838.80	0.52	82-68-8	C6Cl5NO2	293	0.10	0.25	61	1
58	☐	Pentachloronitrobenzene	8.222	249	Unit	178.83	Unit	30	71,494.45	0.52	82-68-8	C6Cl5NO2	293	0.10	0.25	61	1
59	☐	Pentachloronitrobenzene	8.222	214	Unit	141.93	Unit	40	65,750.40	0.48	82-68-8	C6Cl5NO2	293	0.10	0.25	61	1
60	☐	Pentachloronitrobenzene	8.222	235	Unit	140.84	Unit	30	55,327.99	0.40	82-68-8	C6Cl5NO2	293	0.10	0.25	61	1
61	☐	Pentachloronitrobenzene	8.222	237	Unit	118.8	Unit	30	48,606.93	0.35	82-68-8	C6Cl5NO2	293	0.10	0.25	61	1
62	☐	Pentachloronitrobenzene	8.222	235	Unit	116.87	Unit	35	47,530.55	0.35	82-68-8	C6Cl5NO2	293	0.10	0.25	61	1
63	☐	Pentachloronitrobenzene	8.222	237	Unit	166.76	Unit	40	32,421.70	0.24	82-68-8	C6Cl5NO2	293	0.10	0.25	61	1
64	☐	Pentachloronitrobenzene	8.222	237	Unit	140.7	Unit	30	30,650.62	0.22	82-68-8	C6Cl5NO2	293	0.10	0.25	61	1
65	☐	Pentachloronitrobenzene	8.222	235	Unit	164.87	Unit	40	30,475.77	0.22	82-68-8	C6Cl5NO2	293	0.10	0.25	61	1
66	☐	Pentachloronitrobenzene	8.222	295	Unit	264.65	Unit	5	29,999.50	0.22	82-68-8	C6Cl5NO2	293	0.10	0.25	61	1
67	☐	Pentachloronitrobenzene	8.222	295	Unit	142.73	Unit	50	14,185.30	0.10	82-68-8	C6Cl5NO2	293	0.10	0.25	61	1

Figure 7A. Results of MRM transition optimization in the expanded view (A).

B

Optimized MRM Transitions — Select number of top ranked transitions: 5 — Left RT Delta (min): 0.20 — Right RT delta (min): 0.20 — Overwrite RT Delta — Nested View

	Compound Name	RT (min)	Left RT Delta (min)	Right RT delta (min)	CAS #	Formula	Molecular Weight	Sample Position	Injection Volume (µL)
⊞ 1	Novaluron	5.338	0.10	0.20	116714-46-6	C17H9ClF8N2O4	492	61	1
⊞ 2	Etridiazole	5.833	0.10	0.19	2593-15-9	C5H5Cl3N2OS	246	61	1
⊞ 3	Ethoprophos	7.012	0.10	0.32	13194-48-4	C8H19O2PS2	242	61	1
⊞ 4	Pentachloronitrobenzene	8.222	0.10	0.25	82-68-8	C6Cl5NO2	293	61	1
⊞ 5	Diazinon	8.281	0.10	0.21	333-41-5	C12H21N2O3PS	304	61	1
⊞ 6	Methyl parathion	9.139	0.11	0.21	298-00-0	C8H10NO5PS	263	61	1
⊞ 7	Metalaxyl	9.332	0.12	0.28	57837-19-1	C15H21NO4	279	61	1
⊞ 8	Kinoprene	9.731	0.10	0.22	42588-37-4	C18H28O2	276	61	1
⊞ 9	Fenthion	9.919	0.11	0.24	55-38-9	C10H15O3PS2	278	61	1
⊞ 10	Chlorpyrifos	9.953	0.11	0.21	2921-88-2	C9H11Cl3NO3PS	349	61	1
⊞ 11	MGK 264 (Synergist 264) (Pyrdone)	10.435	0.11	0.25	113-48-4	C17H25NO2	275	61	1
⊞ 12	trans-Chlordane	11.036	0.12	0.13	5103-74-2	C10H6Cl8	406	61	1
⊞ 13	Endosulfan (alpha isomer)	11.269	0.13	0.25	959-98-8	C9H6Cl6O3S	404	61	1
14	cis-Chlordane	11.299	0.18	0.16	5103-71-9	C10H6Cl8	406	61	1
⊞ 15	Kresoxim-methyl	11.821	0.11	0.25	143390-89-0	C18H19NO4	313	61	1
⊞ 16	Chlorfenapyr	12.051	0.11	0.14	122453-73-0	C15H11BrClF3N2O	406	61	1
⊞ 17	Endosulfan (beta isomer)	12.280	0.12	0.27	33213-65-9	C9H6Cl6O3S	404	61	1
⊞ 18	Piperonyl butoxide	13.386	0.12	0.24	51-03-6	C19H30O5	338	61	1
⊞ 19	Bifenthrin	13.931	0.12	0.25	82657-04-3	C23H22ClF3O2	422	61	1
⊞ 20	Bifenazate	13.964	0.21	0.26	149877-41-8	C17H20N2O3	300	61	1
⊞ 21	(1R)-cis-Permethrin	15.632	0.12	0.19	54774-46-8	C21H20Cl2O3	390	61	1
⊞ 22	(1R)-trans-Permethrin	15.751	0.11	0.24	61949-77-7	C21H20Cl2O3	390	61	1
⊞ 23	Pyridaben	15.787	0.11	0.21	96489-71-3	C19H25ClN2OS	364	61	1
⊞ 24	Boscalid (Nicobifen)	16.610	0.13	0.23	188425-85-6	C18H12Cl2N2O	342	61	1
⊞ 25	Dimethomorph-(Z) {CAS # 110488-70-5}	18.495	0.15	0.22	999012-03-2	C21H22ClNO4	387	61	1

Figure 7B. Results of MRM transition optimization in the nested view.

The developed MRM acquisition method can be saved as either a time-segment MRM method or a dMRM method (Figure 8). The user defines minimum dwell time and the number of cycles per second when saving the method. The developed transitions can be also exported as a properly formated .CSV file.

The developed and optimized MRM acquisition method was successfully used for trace-level pesticide quantitation in a challenging cannabis matrix, with the results shown elsewhere.[3]

Conclusion

A highly automated optimization tool for MRM acquisition, MassHunter Optimizer for GC/TQ was used to efficiently develop up to 18 transitions for each of the 25 pesticides of interest, which are regulated in cannabis. The *Start from scan data* workflow was used with manual revision of the precursor identification step. The remaining optimization steps were automated. Collision energies were re-optimized in dried cannabis flower matrix to enhance method selectivity. The optimized results were saved as a time segment or a dMRM method.

C

4	Pentachloronitrobenzene		8.222	0.10	0.25	82-68-8	C6Cl5NO2	293

Precursor Ion	Abundance
295.00	700,222.00

Product Ion	Abundance	%	CE
236.80	94,459.98	1.00	20.00
264.65	29,999.50	0.32	5.00
142.73	14,185.30	0.15	50.00

249.00	1,198,112.00
237.00	2,193,355.00
235.00	1,485,550.00
214.00	1,639,871.00
212.00	1,263,132.00

Figure 7C. Results of MRM transition optimization in the nested view with pentachloronitrobenzene results expanded.

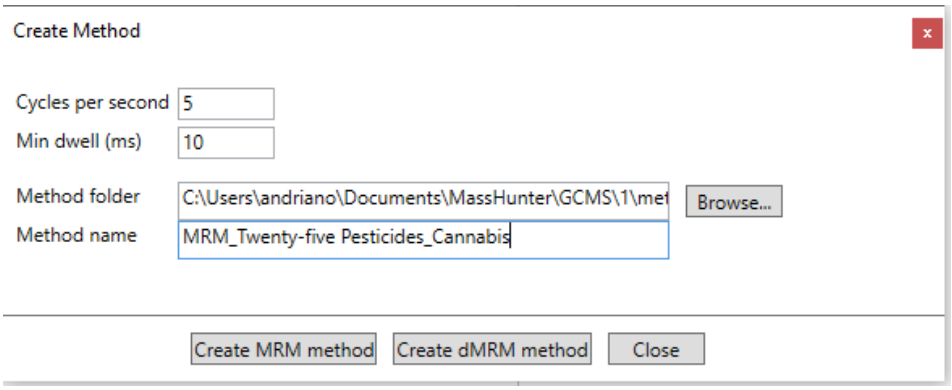


Figure 8. Creating a method with the Agilent MassHunter Optimizer for GC/TQ.

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