



MassHunter Pesticide Personal Compound Database and Library

Method Setup Guide

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Use this guide to create Q-TOF methods to use with your Personal Compound Database and Library (PCDL).

The instructions in this guide are based on the **5190-0551 LC/MS Pesticide Comprehensive Test Mix** (sold separately). The Comprehensive Test Mix is not required, but it can be a helpful tool to develop your own methods.

Before you begin, make sure that your system meets the installation requirements that are described in the *MassHunter Pesticide Personal Compound Database and Library Quick Start Guide*.

For more detailed instructions, see the *Familiarization Guide*, and the MassHunter Data Acquisition for 6500 Series Quadrupole TOF LC/MS *Familiarization Guide* and *online Help*.



Step 1. Set up the LC part of the method

1 Prepare the standards.

The concentration of the test mix stock solution is 100 µg/mL (100 ppm).

a Dilute 10 µL of the stock solution to 1.0 mL with acetonitrile.

For more accurate results, and if conservation of sample is not a concern, dilute 100 µL of the stock solution to 10.0 mL of solvent instead.

b Transfer 1 mL of the final sample solution to a standard 2-mL sample vial for analysis.

The final solution is a 1 µg/mL (1 ppm) working solution.

2 Set up the mobile phases.

This step is identical for all LC modules.

- Solvent A: 5 mM ammonium formate/0.1% formic acid in water
- Solvent B: 5 mM ammonium formate/0.1% formic acid in methanol

3 Check that the method is set up to make a 2-µL injection.

4 Set up the gradient.

The gradient setup is dependent upon the LC configuration. The parameters that follow are examples.

5 Make sure that the Column Compartment temperature is set to 40°C.

Step 1. Set up the LC part of the method

1290 Infinity LC system

1290 Infinity LC system with Agilent Eclipse Plus C18, 2.1 mm × 150 mm, 1.8- μ m ZORBAX LC column (p/n 959759-902), sold separately.

Time [min]	Δ	A [%]	B [%]	Flow [mL/min]	Max. Pressure Limit [bar]
0.00		95.00	5.00	0.400	1200.00
0.50		95.00	5.00	0.400	1200.00
3.50		50.00	50.00	0.400	1200.00
17.00		0.00	100.00	0.400	1200.00
20.00		0.00	100.00	0.400	1200.00
20.10		95.00	5.00	0.400	1200.00

Stop time is 22 minutes with a post time of 2 minutes.

1260 Infinity LC system

The 1260 Infinity LC system can have a lower backpressure limit (up to 600 bar) and a higher dead volume than the 1290 Infinity LC system.

Time [min]	Δ	A [%]	B [%]	Flow [mL/min]	Max. Pressure Limit [bar]
0.00		95.00	5.00	0.400	600.00
▶ 3.50		50.00	50.00	0.400	600.00
17.00		0.00	100.00	0.400	600.00
20.00		0.00	100.00	0.400	600.00
20.10		95.00	5.00	0.400	600.00

Stop time is 22 minutes with a post time of 2 minutes.

Step 2. Set up LC/MS ion source parameters

- Set up the ion source parameters in the MS part of the method tab.
For a multicomponent method, the ion source parameters shown in the next tables are used to achieve the best overall sensitivity for all compounds in the Comprehensive Test Mix. You can adjust the method to optimize for individual compounds or submixes.

Table 1 ESI Ion Source

ESI Ion Source Parameters	6520/6530/6540 Q-TOF LC/MS
Gas Temp (°C)	350
Drying Gas (L/min)	12
Nebulizer (psig)	35
VCap	3500 (Pos), 3000 (Neg)
Fragmentor	120 (Pos), 120 (Neg)
Skimmer	65
OCT 1 RF Vpp	750

Table 2 Dual ESI Ion Source

Dual ESI Ion Source Parameters	6520/6530/6540 Q-TOF LC/MS
Gas Temp (°C)	350
Drying Gas (L/min)	12
Nebulizer (psig)	35
VCap	3500 (Pos), 3000 (Neg)
Fragmentor	120 (Pos), 120 (Neg)
Skimmer	65
OCT 1 RF Vpp	750

Step 2. Set up LC/MS ion source parameters

Table 3 Agilent Jet Stream Ion Source

Agilent Jet Stream Ion Source Parameters	6520/6530/6540 Q-TOF LC/MS	6550/6560 Q-TOF LC/MS
Gas Temp (°C)	120	120
Drying Gas (L/min)	57	15
Nebulizer (psig)	35	35
Sheath Gas Temp (°C)	375	375
Sheath Gas Flow (L/min)	12	12
Capillary (V)	3500 (Pos), 3000 (Neg)	3500 (Pos), 3000 (Neg)
Nozzle Voltage (V)	300 (Pos), 0 (Neg)	300 (Pos), 0 (Neg)
High Pressure RF (V)	N/A	150 (Pos), 90 (Neg)
Low Pressure RF (V)	N/A	60 (Pos), 60 (Neg)
Fragmentor	140	380
Skimmer	65	N/A
OCT 1 RF Vpp	750	750

Nebulizer pressure depends to a large extent on the flow rate that is used. The fragmentor voltage on the non-iFunnel configuration also depends on the molecule size.

Step 3. Set up a worklist to run the submixes

Step 3. Set up a worklist to run the submixes

- Set up the worklist as shown in [Figure 1](#). Include all submixes. Inject the first standard twice to allow the system to come to equilibrium.

	<input checked="" type="checkbox"/>	Sample Name	Sample Position	Method	Data File	Sample Type
1	<input checked="" type="checkbox"/>	SubMix_01	P1-A1	Pesticide_ComprehensiveTestMix.m	todelete.d	Sample
2	<input checked="" type="checkbox"/>	SubMix_01	P1-A1	Pesticide_ComprehensiveTestMix.m	Submix_1.d	Sample
3	<input checked="" type="checkbox"/>	SubMix_02	P1-A2	Pesticide_ComprehensiveTestMix.m	Submix_2.d	Sample
4	<input checked="" type="checkbox"/>	SubMix_03	P1-A3	Pesticide_ComprehensiveTestMix.m	Submix_3.d	Sample
5	<input checked="" type="checkbox"/>	SubMix_04	P1-A4	Pesticide_ComprehensiveTestMix.m	Submix_4.d	Sample
6	<input checked="" type="checkbox"/>	SubMix_05	P1-A5	Pesticide_ComprehensiveTestMix.m	Submix_5.d	Sample
7	<input checked="" type="checkbox"/>	SubMix_06	P1-A6	Pesticide_ComprehensiveTestMix.m	Submix_6.d	Sample
8	<input checked="" type="checkbox"/>	SubMix_07	P1-A7	Pesticide_ComprehensiveTestMix.m	Submix_7.d	Sample
9	<input checked="" type="checkbox"/>	SubMix_08	P1-A8	Pesticide_ComprehensiveTestMix.m	Submix_8.d	Sample

Figure 1 Worklist

For more information about Q-TOF methods, refer to the *Familiarization Guide* for this database, or the MassHunter Data Acquisition for 6500 Series Quadrupole TOF LC/MS *Familiarization Guide* or *online Help*.

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In this Book

The *Method Setup Guide* describes how to create methods for your specific LC/MS setup. The methods can be used with the Comprehensive Test Mix.

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