

Separation Times



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Hybrid Quadrupole/Time-of-Flight (Q-TOF) LC/MS for the screening and confirmation of pesticides

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There are a plethora of pesticides in use throughout the world, and you need analytical tools that can provide high sensitivity and selectivity along with a full scope of applicability to identify those pesticides – especially at the low levels of concern. Here’s how Agilent’s [Hybrid Quadrupole/Time-of-Flight LC/MS \(Q-TOF LC/MS\)](#) system meets these needs.

Using a target list of compounds, you can readily screen by MS/MS with triple quadrupole technology [1]. It is not easy to compare the duty cycle for MS/MS using Q-TOF to an equivalent approach because of the pulsed full spectra attribute of the technology. However, the very fact that the time-of-flight technology always gives you full mass spectra lets you screen massive numbers of compounds using database searches by molecular formula or exact masses [2].

Name	RT	Mass	Molwt	Formula	Sp Mass	Diff (ppm)	DB Formula	DB Diff(ppm)	Sim (%)
Cap 527 Fenoxazole	6.9	374.1528	368	C22H18N2O4	374.1265	-1.01	C22H18N2O4	1.01	5
Cap 226 Spiroxamine	11	287.2687	278	C18H23N2O2	287.2615	-0.21	C18H23N2O2	0.21	5
Cap 235 Imidacloprid	14	281.1438	262	C10H9ClN2O2	267.0616	6.54	C10H9ClN2O2	6.54	5
Cap 81 Imidacloprid	15	282.1548	266	C10H9N2O2	262.0668	1.74	C10H9N2O2	1.74	5

Table 1. Results of a database search of fruit extract. Four compounds were found with no retention time specified in the database. ([Click here](#) to see this image larger.)

m/z 100 and 20,000 at m/z 1500. Plus, you can obtain sensitivity as low as 1 pg on-column for some pesticides. **Table 1** shows the results of a screen in a fruit extract.

In addition to using a simple spreadsheet in .csv format to create an automatically searchable database, Agilent now offers a 1300 plus pesticide database in [Metlin format](#), complete with structures and other useful information.

Even with accurate mass, a recent evaluation showed that two ions are necessary for confirmation [3]. So you can identify compounds in the screening step using single MS, and then target them again in MS/MS mode for confirmation. The Agilent Q-TOF provides sensitive MS/MS with full spectra containing the accurate mass of each fragment. This allows you to correlate each fragment with the proposed precursor molecular formula, so that, you can state with a high degree of confidence whether or not the detected compound is the same compound identified in the database search.

Figure 1 shows an example of this process. In this example the identified compound, spiroxamine, is confirmed with the accurate mass fragments.

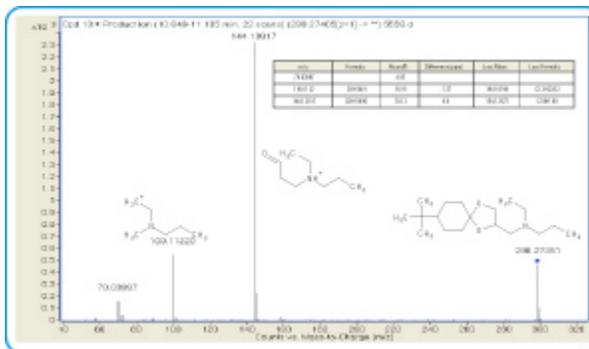


Figure 1. The MS/MS spectrum is shown for the tentatively identified spiroxamine, using the “Find Targeted MS/MS” tool in [MassHunter software](#). Note that only formulas matching the proposed precursor ion formula are given by the software, as shown in the table. ([Click here](#) to see this image larger.)

Comparing the full MS/MS spectrum to that of an authentic standard that has the same

chromatographic retention time provides unambiguous confirmation. Quantification on the Q-TOF is also practical because of the high dynamic range afforded by both the 4GHz sampling and analog to digital conversion of the acquisition electronics. These capabilities are exemplified in recently published applications notes. [5-7] Quantitation of a large number of compounds is still best performed on the Agilent LC/MS Triple Quadrupole.

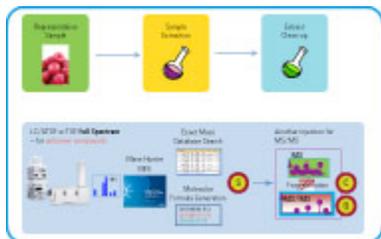


Figure 2. Workflow for pesticide analysis with Agilent Q-TOF. ([Click here](#) to see this image larger.)

Figure 2 shows a summary of the pesticide workflow using the Agilent Q-TOF LC/MS for identification and confirmation for targeted and non-targeted compounds. Because of the high selectivity, a simple extraction procedure such as QuEChERS [4] is all that is needed. Screening is performed in the single MS mode using a large database to search for anticipated and unexpected use of pesticides. Confirmation is made using targeted MS/MS of the found compounds. Typically, only a few pesticides will be found in any given commodity and these can readily be quantified on the Q-TOF.

The Agilent LC/MS Q-TOF provides:

- High selectivity produced by accurate mass measurement and high resolving power
- High sensitivity in single MS and MS/MS modes for screening and confirmation
- Highly selective quantitation

To learn more about how you can increase your confidence in your results and improve your overall productivity with [Agilent's 6500 Series Accurate-Mass Q-TOF LC/MS](#), visit our product page or contact your Agilent Representative.

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