

A reliable and routine LC/MS/MS Screening of Multiclass PGRs in Grapes using Agilent Q-TOF LC/MS coupled with an Agilent Infinity LC

FOOD SAFETY



The Agilent 6530 Accurate Mass Q-TOF LC/MS System provides high sensitivity with outstanding mass accuracy and resolution and simple, fast, and economic sample cleanup for simultaneous screening of multiclass PGRs in grapes



Plant hormones, or phytohormones, are chemicals that regulate plant growth. Manmade compounds called PGRs are used to regulate growth of cultivated plants, weeds, and plants and plant cells grown in vitro. There are five major classes: abscisic acid, auxins, cytokinins, ethylene, and gibberellins. PGRs activate cellular response including cell death. Some can adversely affect human cancer cells. European Union testing labs found chlormequat in imported grapes from India, which triggered additional testing for PGRs. Multiresidue monitoring of PGRs is challenging due to the diversity of their chemical properties. These compounds are thermally unstable and therefore not amenable to gas chromatographic analysis without derivatization. Matrix co-extractives interfere with the target HPLC-UV signals, lowering the sensitivity of PGR analysis by high performance liquid chromatography (HPLC). Moderate to high aqueous solubility restricts multiresidue recovery by phase separation with organic solvents and makes the sample cleanup difficult due to variable affinity of different PGRs towards different cleanup agents or adsorbents.

This note describes the simple, fast, and economic sample cleanup process and targeted MS/MS scan for simultaneous screening of multiclass PGRs in grape samples.

The Approach

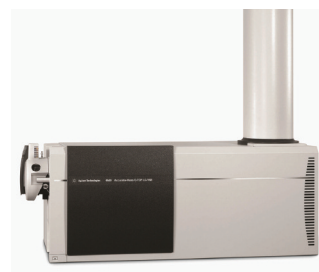
An Agilent 1290 Infinity LC with an Agilent ZORBAX Rapid Resolution High Definition (RRHD) column and an Agilent ZORBAX Extended C18 column interfaced to the Agilent 6530 Accurate-Mass Q-TOF LC/MS system provided excellent retention time reproducibility, outstanding mass accuracy, and the resolution required for the screening of multiclass PGRs in grapes.

Compounds

- Chlormequat, Daminozide, Zeatin, Kinetin, 6-BA, IAA, IBA, Forchlorfenuron, Paclobutrazol, GA3, ABA, 2-4-D, and d4-Chlormequat as ISTD

Key Benefits

- Results shows very good sensitivity with outstanding mass accuracy and resolution for screening of PGRs using Agilent 6530 Accurate-Mass Q-TOF LC/MS with Jetstream ESI ion source and Agilent 1290 Infinity LC
- Simple, economic and rugged sample cleanup using Dispersive C18 ODS bulk without any derivatization process
- Simultaneous screening of Multiclass PGRs without sacrificing sensitivity
- Better than 5 ppm mass accuracy/more than 20,000 resolution helps to identify targeted compounds, and automated MFE helps to generate molecular formula for unknown compounds from a complex matrix such as grapes.



Screening of Multiclass PGRs in Grapes Using Agilent Q-TOF LC/MS/MS Coupled with an Agilent 1290 Infinity LC

Figure 1 shows good chromatographic separation of nine PGRs in positive mode and three PGRs in negative mode. Mass accuracy for all standards in scan mode is within 5 ppm for standards at ppb level concentration.

Figure 2 shows the mass accuracy for all standards. Dispersive C18 sample cleanup techniques show good sample cleanup to remove matrix. Outstanding mass accuracy and resolution helped to identify PGRs even at ppb level concentration from grape matrix. Figure 3 shows mass accuracy for all standards spiked and extracted from grape samples.

Summary

The Agilent 6530 Accurate-Mass Q-TOF LC/MS system with Jetstream ESI ion source coupled with an Agilent 1290 Infinity LC and Dispersive C18 ODS sample cleanup shows excellent sensitivity, mass accuracy, and resolution for simultaneous screening of multiclass PGRs in grapes.

Acknowledgment

Grape samples were provided by the National Research Center for Grapes, Pune, India. Project work was carried out in collaboration with Dr. Kaushik Banerjee- Sr Scientist from NRCG, Pune, India.

Reference

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2. Michael Zumwalt, David Weil, Chin-Kai Meng, "The use of Accurate-mass, Isotope Ratios and MS/MS for the PPCPs in Water."

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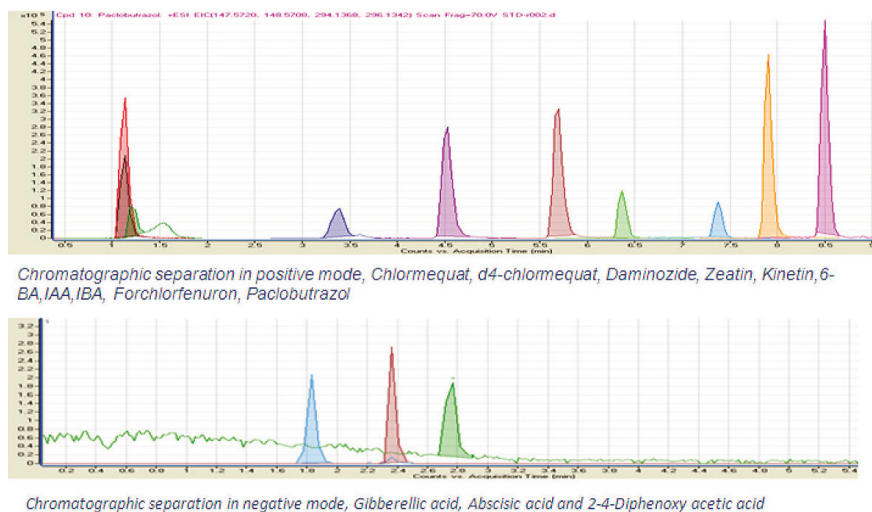


Figure 1. Good chromatographic separation of nine PGRs in positive mode and three PGRs in negative mode.

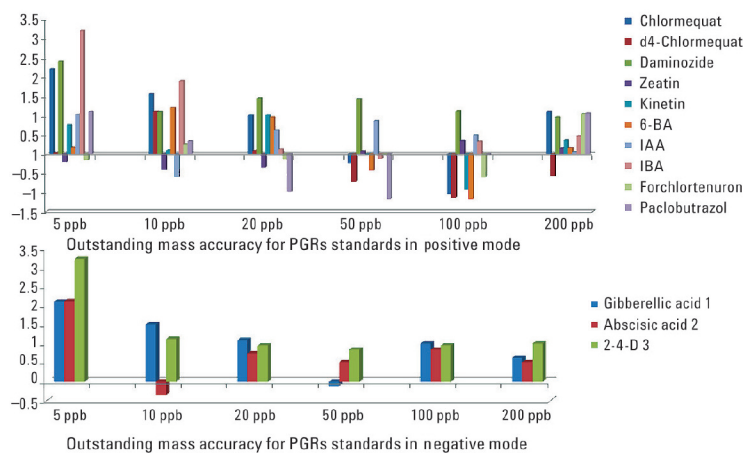


Figure 2. Outstanding mass accuracy for standards in positive and negative mode.

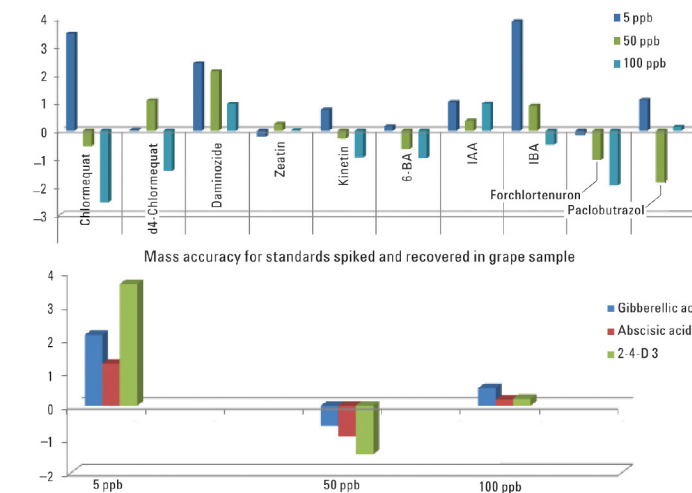


Figure 3. Outstanding mass accuracy for standards spiked and extracted from grape matrix.



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