

# Qualitative Comparison of Wine Process Samples with UHPLC and Ultra-High Resolution TOFMS

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### ABSTRACT

The evaluation, identification, and quantitation of flavones, antioxidants and related nutrients, biogenic amines, and potential contaminants in wine and other foodstuffs provides valuable information on their nutritional and health values. The transition of winemaking from an art to a more exacting science is dependent upon the detection and understanding of nutrient and flavor loss and accumulation during the processing. In addition, the ability to detect and quantify potential contaminant compounds such as biogenic amines, pesticides, herbicides, fungicides, and phytotoxins is also of critical importance. In the present study, ultra-high resolution TOFMS with multiple reflections was utilized to generate fingerprints of several wines and their pre-harvest wine grape juices.

#### EXPERIMENTAL METHOD

A UHPLC method for analysis of wine samples was developed on the Citius<sup>™</sup> LC-HRT. This system permits resolutions up to 100,000 with high mass accuracy (< 1 ppm). An ESI interface was used for sample ionization in positive ion mode. Data files were searched for a list of 90+ flavones, antioxidants, biogenic amines, pesticides, herbicides, fungicides, and phytotoxins. Data were also evaluated for non-targeted compounds. Paired sets of pre-harvest grape juice and the corresponding wine were analyzed for a number of wine varietals and differential concentrations and the responsible compounds identified.

An Agilent UHPLC was utilized at the following conditions:

LC Agilent 1290 Infinity

Column 1.8 µm HSS T3 100 mm x 1.0 mm ID

Mobile Phase A: 0.1% formic acid and 0.01% ammonia in water

B: Acetonitrile

Flow 0.120 mL/min

Gradient 0% (1st min); 0% to 7.5% (1-4 min); 7.5% to 97.5%

(4-16 min); 97.5% (16-22 min); 0% (22.2-26.2 min)

Column Temperature 35°

Injection Volume Typ. 7.5 µL, although other volumes/dilutions

were used as well

Samples 5 pair of wine grape juice and finished wines (Vidal Blanc,

Am. Riesling, Cabernet, Franc Rose, Cabernet Franc, Syrah)

Mass Spectrometer LECO CITIUS™ LC-HRT

Ion Source LECO ESI

Polarity Positive

Acquisition Mode High Resolution – 20 m (1-FFP™ Pass)

Mass Resolution Typically 50,000 FWHM (asymptotic)

Spectral Acquisition 2.5-10 spectra/second

m/z Range 50-2250

m/z Calibration Optional 10 s programmed co-infusion

at end of run; using calibrant delivery module (CDM)

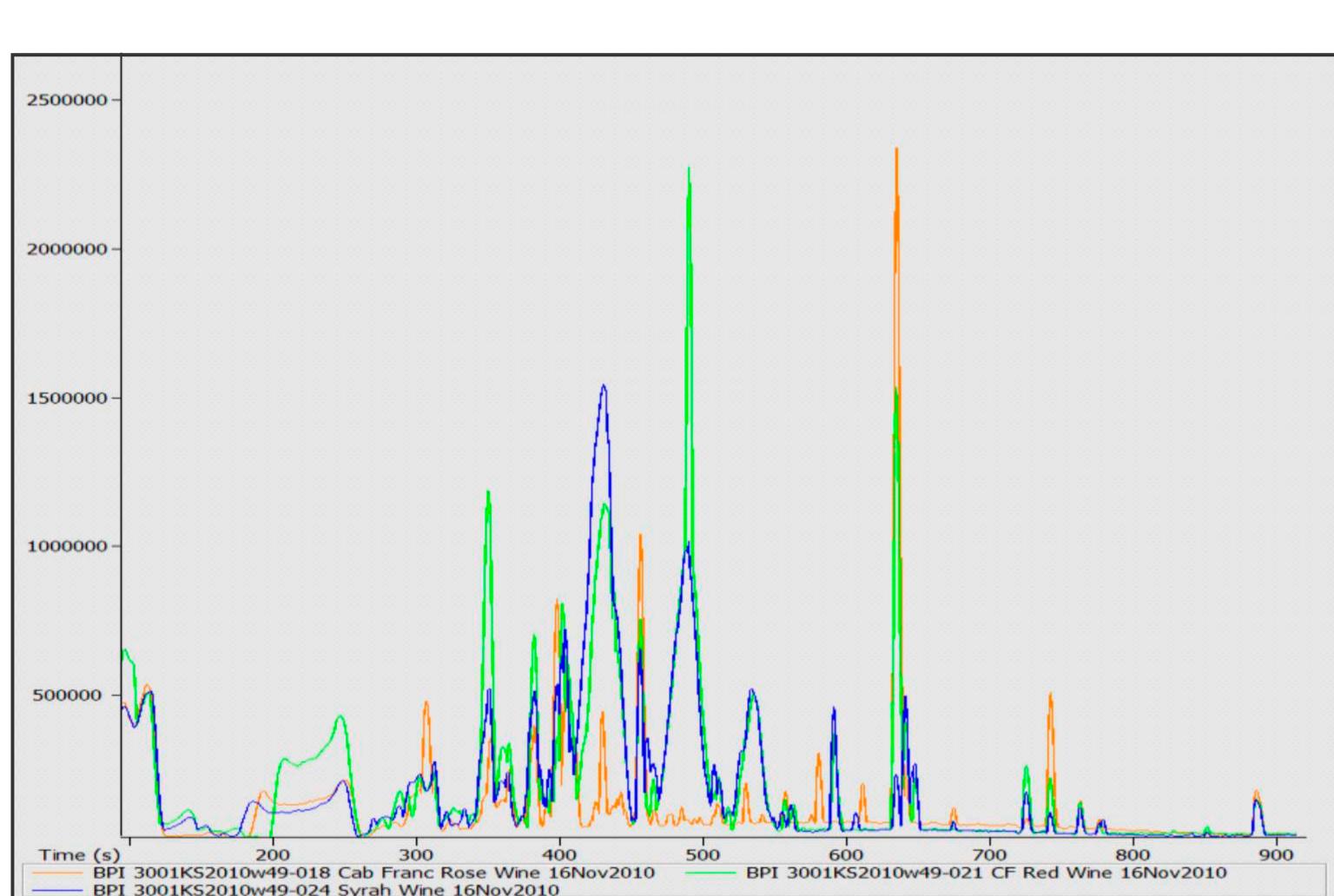
and Agilent tune mix

## RESULTS

The evaluation, identification, and quantitation of flavones, antioxidants and related nutrients, biogenic amines, and potential contaminants in wine and other foodstuffs provides valuable information on their nutritional and health values. The transition of winemaking from an art to a more exacting science is dependent upon the detection and

A variety of polyphenolic compounds were detected including flavan-3-ols ((epi)catechin)) and flavanols (kaempferol, quercetin, myricetin). The major contributors to the total antioxidant status were organic acids (coumaric acid, vanillic acid, and syringic acid), and resveratrol. The relative levels varied with the different wine varietals.

Many pesticides were also observed in the grape juice and wine samples with higher response levels for pyrimethanil in select varietals. Also observed were tebuconazole, boscalid, and fenhexamid. Interestingly, the relative levels of pesticides in the matched red grape juice and wine pairs were generally higher in the wine vs. the juice, although the relative enhancements varied by 1.1 fold to 100 fold depending on the pesticide and the wine type. An example of the Bass Peak Intensity (BPI chromatogram) is presented below for the red wines.





## LIST OF FORMULAE SEARCH CANDIDATES

Biogenic Amines

94.0651 103.123 112.0869	$C_6H_7N$	2-Phenylamine	Biogenic Amines
	$C_5H_{14}N_2$	Cadaverine	Biogenic Amines
	$C_5H_9N_3$	Histamine	Biogenic Amines
122.0964	C <sub>8</sub> H <sub>11</sub> N	2-Phenylethylamine	Biogenic Amines
136.0757	C <sub>8</sub> H <sub>9</sub> NO	UTA (o-aminoacetophenone)	Un/Atypical Aging
138.0913	C <sub>8</sub> H <sub>11</sub> NO	Tyramine	Biogenic Amines
146.1652	$C_7H_{19}N_3$	Spermidine	Biogenic Amines
166.0863	$C_9H_{11}NO_2$	Metholcarb	Pesticides
155.0339	C <sub>7</sub> H <sub>6</sub> O <sub>4</sub>	Dihydroxybenzoic acid	Antioxidants
161.1073	$C_{10}H_{12}N_2$	Tryptamine	Biogenic Amines
165.0546	$C_9H_8O_3$	Coumaric acid	Antioxidants
169.0495	C <sub>8</sub> H <sub>8</sub> O <sub>4</sub>	Vanillic acid	Antioxidants
171.0288	$C_7H_6O_5$	Gallic acid	Antioxidants
181.0495	C <sub>9</sub> H <sub>8</sub> O <sub>4</sub>	Caffeic acid	Antioxidants
192.0768	$C_9H_9N_3O_2$	Carbendazim	Pesticides*
194.1176	$C_{11}H_{15}NO_2$	Isoprocarb	Pesticides
195.0652	C <sub>10</sub> H <sub>10</sub> O <sub>4</sub>	Ferulic acid	Antioxidants
199.0601	$C_9H_{10}O_5$	Syringic acid	Antioxidants
199.0826	$C_7H_{10}N_4O_3$	Cymoxanil	Pesticides
200.1182	$C_{12}H_{13}N_3$	Pyrimethanil	Pesticides
202.0863	$C_{12}H_{11}NO_2$	Carbaryl	Pesticides
203.223	$C_{10}H_{26}N_4$	Spermine	Biogenic Amines
208.1332	$C_{12}H_{17}NO_2$	Fenobucarb	Pesticides
210.1125	$C_{11}H_{15}NO_3$	Propoxur	Pesticides
220.075	$C_7H_{13}N_3O_3S$	Oxamyl	Pesticides
222.1125	$C_{12}H_{15}NO_3$	Carbofuran	Pesticides
223.0745	C <sub>10</sub> H <sub>11</sub> CIN <sub>4</sub>	Acetamiprid	Pesticides
225.0757	$C_{11}H_{12}O_5$	Sinapic acid	Antioxidants
226.0896	$C_{11}H_{15}NO_2S$	Methiocarb	Pesticides
226.0896	$C_{11}H_{15}NO_2S$	Ethiofencarb	Pesticides
226.1339	$C_{14}H_{15}N_3$	Cyprodinil	Pesticides
229.0859	$C_{14}H_{12}O_3$	Resveratrol	Antioxidants
230.0069	C <sub>5</sub> H <sub>12</sub> NO <sub>3</sub> PS <sub>2</sub>	Dimethoate	Pesticides
239.1503	C <sub>11</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub>	Pirimicarb	Pesticides
249.047	$C_{12}H_6F_2N_2O_2$	Fludioxonil	Pesticides
256.0596	$C_9H_{10}CIN_5O_2$	Imidacloprid	Pesticides
258.0714	C <sub>12</sub> H <sub>16</sub> CINOS	Thiobencarb	Pesticides
264.009	$C_8H_{10}NO_5PS$	Parathion-methyl	Pesticides
268.1543	C <sub>14</sub> H <sub>21</sub> NO <sub>4</sub>	Diethofencarb	Pesticides
278.0247	$C_9H_{12}NO_5PS$	Fenitrothion	Pesticides
280.1543	$C_{15}H_{21}NO_4$	Metalaxyl	Pesticides
284.024	$C_{13}H_{11}CI_2NO_2$	Procymidone	Pesticides
284.0716	$C_{13}H_{15}CI_2N_3$	Penconazole	Pesticides
287.055	$C_{15}H_{10}O_6$	Kaempferol	Flavanol
289.1215	$C_{15}H_{17}CIN_4$	Myclobutanil	Pesticides
291.0863	C <sub>15</sub> H <sub>14</sub> O <sub>6</sub>	(epi) catechin	Flavanol
294.1004	$C_{14}H_{16}CIN_3O_2$	Triadimefon	Pesticides
296.116	C <sub>14</sub> H <sub>18</sub> CIN <sub>3</sub> O <sub>2</sub>	Triadimenol	Pesticides
298.2741	C <sub>18</sub> H <sub>35</sub> NO <sub>2</sub>	Spiroxamine	Pesticides
330.0407	$C_{13}H_{13}CI_2N_3O_3$	Iprodione	Pesticides
301.0505	$C_{13}H_{11}CI_2NO_2$	Procymidone (M+NH <sub>4</sub> ) <sup>+</sup>	Pesticides
302.0709	$C_{14}H_{17}CI_2NO_2$	Fenhexamid	Pesticides
302.1387	C <sub>17</sub> H <sub>19</sub> NO <sub>4</sub>	Fenoxycarb	Pesticides
		Ellagic acid	A 11 1 1 -
	$C_{14}H_6O_8$		Antioxidants
303.0135	$C_{14}H_6O_8$ $C_{15}H_{10}O_7$	Quercetin	Flavanol
303.0135 303.0499			
303.0135 303.0499 308.004	$C_{15}H_{10}O_{7}$	Quercetin	Flavanol
303.0135 303.0499 308.004 308.1524	$C_{15}H_{10}O_{7}$ $C_{15}H_{8}CI_{2}FNO$	Quercetin Quinoxyfen	Flavanol Pesticides
303.0135 303.0499 308.004 308.1524 312.1165	$C_{15}H_{10}O_{7}$ $C_{15}H_{8}CI_{2}FNO$ $C_{16}H_{22}CIN_{3}O$	Quercetin Quinoxyfen Tebuconazole	Pesticides Pesticides
303.0135 303.0499 308.004 308.1524 312.1165 314.1387	$C_{15}H_{10}O_{7}$ $C_{15}H_{8}CI_{2}FNO$ $C_{16}H_{22}CIN_{3}O$ $C_{17}H_{17}N_{3}OS$	Quercetin Quinoxyfen Tebuconazole Fenamidone	Pesticides Pesticides Pesticides
303.0135 303.0499 308.004 308.1524 312.1165 314.1387	$C_{15}H_{10}O_{7}$ $C_{15}H_{8}CI_{2}FNO$ $C_{16}H_{22}CIN_{3}O$ $C_{17}H_{17}N_{3}OS$ $C_{18}H_{19}NO_{4}$	Quercetin Quinoxyfen Tebuconazole Fenamidone Kresoxim-methyl	Pesticides Pesticides Pesticides Pesticides Pesticides
303.0135 303.0499 308.004 308.1524 312.1165 314.1387 316.1076	$C_{15}H_{10}O_{7}$ $C_{15}H_{8}CI_{2}FNO$ $C_{16}H_{22}CIN_{3}O$ $C_{17}H_{17}N_{3}OS$ $C_{18}H_{19}NO_{4}$ $C_{16}H_{15}F_{2}N_{3}Si$	Quercetin Quinoxyfen Tebuconazole Fenamidone Kresoxim-methyl Flusilazole	Pesticides Pesticides Pesticides Pesticides Pesticides Pesticides Pesticides
303.0135 303.0499 308.004 308.1524 312.1165 314.1387 316.1076 319.0448	$C_{15}H_{10}O_{7}$ $C_{15}H_{8}CI_{2}FNO$ $C_{16}H_{22}CIN_{3}O$ $C_{17}H_{17}N_{3}OS$ $C_{18}H_{19}NO_{4}$ $C_{16}H_{15}F_{2}N_{3}Si$ $C_{15}H_{10}O_{8}$	Quercetin Quinoxyfen Tebuconazole Fenamidone Kresoxim-methyl Flusilazole Myricetin	Flavanol Pesticides Pesticides Pesticides Pesticides Pesticides Flavanol
303.0135 303.0499 308.004 308.1524 312.1165 314.1387 316.1076 319.0448 321.2173	$C_{15}H_{10}O_{7}$ $C_{15}H_{8}CI_{2}FNO$ $C_{16}H_{22}CIN_{3}O$ $C_{17}H_{17}N_{3}OS$ $C_{18}H_{19}NO_{4}$ $C_{16}H_{15}F_{2}N_{3}Si$ $C_{15}H_{10}O_{8}$ $C_{18}H_{28}N_{2}O_{3}$	Quinoxyfen Tebuconazole Fenamidone Kresoxim-methyl Flusilazole Myricetin Iprovalicarb	Flavanol Pesticides Pesticides Pesticides Pesticides Pesticides Flavanol Pesticides
303.0135 303.0499 308.004 308.1524 312.1165 314.1387 316.1076 319.0448 321.2173 326.1751 331.0399	$C_{15}H_{10}O_{7}$ $C_{15}H_{8}CI_{2}FNO$ $C_{16}H_{22}CIN_{3}O$ $C_{17}H_{17}N_{3}OS$ $C_{18}H_{19}NO_{4}$ $C_{16}H_{15}F_{2}N_{3}Si$ $C_{15}H_{10}O_{8}$ $C_{18}H_{28}N_{2}O_{3}$ $C_{20}H_{23}NO_{3}$	Quercetin Quinoxyfen Tebuconazole Fenamidone Kresoxim-methyl Flusilazole Myricetin Iprovalicarb Benalaxyl	Flavanol Pesticides Pesticides Pesticides Pesticides Pesticides Flavanol Pesticides Pesticides
303.0135 303.0499 308.004 308.1524 312.1165 314.1387 316.1076 319.0448 321.2173 326.1751 331.0399 334.1681	$C_{15}H_{10}O_{7}$ $C_{15}H_{8}CI_{2}FNO$ $C_{16}H_{22}CIN_{3}O$ $C_{17}H_{17}N_{3}OS$ $C_{18}H_{19}NO_{4}$ $C_{16}H_{15}F_{2}N_{3}Si$ $C_{15}H_{10}O_{8}$ $C_{18}H_{28}N_{2}O_{3}$ $C_{20}H_{23}NO_{3}$ $C_{17}H_{12}CI_{2}N_{2}O$	Quercetin Quinoxyfen Tebuconazole Fenamidone Kresoxim-methyl Flusilazole Myricetin Iprovalicarb Benalaxyl Fenarimol	Flavanol Pesticides Pesticides Pesticides Pesticides Pesticides Flavanol Pesticides Pesticides Pesticides Pesticides
303.0135 303.0499 308.004 308.1524 312.1165 314.1387 316.1076 319.0448 321.2173 326.1751 331.0399 334.1681 343.0399	$\begin{array}{c} C_{15}H_{10}O_{7} \\ C_{15}H_{8}CI_{2}FNO \\ C_{16}H_{22}CIN_{3}O \\ C_{17}H_{17}N_{3}OS \\ C_{18}H_{19}NO_{4} \\ C_{16}H_{15}F_{2}N_{3}Si \\ C_{15}H_{10}O_{8} \\ C_{18}H_{28}N_{2}O_{3} \\ C_{20}H_{23}NO_{3} \\ C_{17}H_{12}CI_{2}N_{2}O \\ C_{18}H_{24}CIN_{3}O \end{array}$	Quercetin Quinoxyfen Tebuconazole Fenamidone Kresoxim-methyl Flusilazole Myricetin Iprovalicarb Benalaxyl Fenarimol Tebufenpyrad	Flavanol Pesticides Pesticides Pesticides Pesticides Pesticides Flavanol Pesticides Pesticides Pesticides Pesticides Pesticides Pesticides
303.0135 303.0499 308.004 308.1524 312.1165 314.1387 316.1076 319.0448 321.2173 326.1751 331.0399 334.1681 343.0399	$\begin{array}{c} C_{15}H_{10}O_{7} \\ C_{15}H_{8}CI_{2}FNO \\ C_{16}H_{22}CIN_{3}O \\ C_{17}H_{17}N_{3}OS \\ C_{18}H_{19}NO_{4} \\ C_{16}H_{15}F_{2}N_{3}Si \\ C_{15}H_{10}O_{8} \\ C_{18}H_{28}N_{2}O_{3} \\ C_{20}H_{23}NO_{3} \\ C_{17}H_{12}CI_{2}N_{2}O \\ C_{18}H_{24}CIN_{3}O \\ C_{18}H_{12}CI_{2}N_{2}O \end{array}$	Quercetin Quinoxyfen Tebuconazole Fenamidone Kresoxim-methyl Flusilazole Myricetin Iprovalicarb Benalaxyl Fenarimol Tebufenpyrad Boscalid	Flavanol Pesticides Pesticides Pesticides Pesticides Pesticides Flavanol Pesticides Pesticides Pesticides Pesticides Pesticides Pesticides Pesticides Pesticides
303.0135 303.0499 308.004 308.1524 312.1165 314.1387 316.1076 319.0448 321.2173 326.1751 331.0399 334.1681 343.0399 343.0529 346.9852	$\begin{array}{c} C_{15}H_{10}O_{7} \\ C_{15}H_{8}CI_{2}FNO \\ C_{16}H_{22}CIN_{3}O \\ C_{17}H_{17}N_{3}OS \\ C_{18}H_{19}NO_{4} \\ C_{16}H_{15}F_{2}N_{3}Si \\ C_{15}H_{10}O_{8} \\ C_{18}H_{28}N_{2}O_{3} \\ C_{20}H_{23}NO_{3} \\ C_{17}H_{12}CI_{2}N_{2}O \\ C_{18}H_{24}CIN_{3}O \\ C_{18}H_{12}CI_{2}N_{2}O \\ C_{18}H_{14}N_{4}O_{4}S_{2} \\ \end{array}$	Quinoxyfen Tebuconazole Fenamidone Kresoxim-methyl Flusilazole Myricetin Iprovalicarb Benalaxyl Fenarimol Tebufenpyrad Boscalid Thiophanat-methyl	Flavanol Pesticides Pesticides Pesticides Pesticides Pesticides Pesticides Flavanol Pesticides
303.0135 303.0499 308.004 308.1524 312.1165 314.1387 316.1076 319.0448 321.2173 326.1751 331.0399 334.1681 343.0399 343.0529 346.9852 353.2224	$\begin{array}{c} C_{15}H_{10}O_{7} \\ C_{15}H_{8}CI_{2}FNO \\ C_{16}H_{22}CIN_{3}O \\ C_{17}H_{17}N_{3}OS \\ C_{18}H_{19}NO_{4} \\ C_{16}H_{15}F_{2}N_{3}Si \\ C_{15}H_{10}O_{8} \\ C_{18}H_{28}N_{2}O_{3} \\ C_{20}H_{23}NO_{3} \\ C_{17}H_{12}CI_{2}N_{2}O \\ C_{18}H_{24}CIN_{3}O \\ C_{18}H_{12}CI_{2}N_{2}O \\ C_{18}H_{12}CI_{2}N_{2}O \\ C_{18}H_{12}CI_{2}N_{2}O \\ C_{19}H_{14}N_{4}O_{4}S_{2} \\ C_{10}H_{13}CI_{2}FN_{2}O_{2}S_{2} \\ \end{array}$	Quercetin  Quinoxyfen  Tebuconazole  Fenamidone  Kresoxim-methyl  Flusilazole  Myricetin  Iprovalicarb  Benalaxyl  Fenarimol  Tebufenpyrad  Boscalid  Thiophanat-methyl  Tolyfluanid	Flavanol Pesticides Pesticides Pesticides Pesticides Pesticides Pesticides Flavanol Pesticides
303.0135 303.0499 308.004 308.1524 312.1165 314.1387 316.1076 319.0448 321.2173 326.1751 331.0399 334.1681 343.0399 343.0529 346.9852 353.2224 354.8915	$\begin{array}{c} C_{15}H_{10}O_{7} \\ C_{15}H_{8}CI_{2}FNO \\ C_{16}H_{22}CIN_{3}O \\ C_{17}H_{17}N_{3}OS \\ C_{18}H_{19}NO_{4} \\ C_{16}H_{15}F_{2}N_{3}Si \\ C_{15}H_{10}O_{8} \\ C_{18}H_{28}N_{2}O_{3} \\ C_{20}H_{23}NO_{3} \\ C_{17}H_{12}CI_{2}N_{2}O \\ C_{18}H_{24}CIN_{3}O \\ C_{18}H_{12}CI_{2}N_{2}O \\ C_{18}H_{12}CI_{2}N_{2}O \\ C_{12}H_{14}N_{4}O_{4}S_{2} \\ C_{10}H_{13}CI_{2}FN_{2}O_{2}S_{2} \\ C_{22}H_{28}N_{2}O_{2} \end{array}$	Quinoxyfen Tebuconazole Fenamidone Kresoxim-methyl Flusilazole Myricetin Iprovalicarb Benalaxyl Fenarimol Tebufenpyrad Boscalid Thiophanat-methyl Tolyfluanid Tebufenozide	Flavanol Pesticides Pesticides Pesticides Pesticides Pesticides Pesticides Flavanol Pesticides
303.0135 303.0499 308.004 308.1524 312.1165 314.1387 316.1076 319.0448 321.2173 326.1751 331.0399 334.1681 343.0399 343.0529 346.9852 353.2224 354.8915	$\begin{array}{c} C_{15}H_{10}O_{7} \\ C_{15}H_{8}CI_{2}FNO \\ C_{16}H_{22}CIN_{3}O \\ C_{17}H_{17}N_{3}OS \\ C_{18}H_{19}NO_{4} \\ C_{16}H_{15}F_{2}N_{3}Si \\ C_{15}H_{10}O_{8} \\ C_{18}H_{28}N_{2}O_{3} \\ C_{20}H_{23}NO_{3} \\ C_{17}H_{12}CI_{2}N_{2}O \\ C_{18}H_{24}CIN_{3}O \\ C_{18}H_{12}CI_{2}N_{2}O \\ C_{18}H_{12}CI_{2}N_{2}O \\ C_{12}H_{14}N_{4}O_{4}S_{2} \\ C_{10}H_{13}CI_{2}FN_{2}O_{2}S_{2} \\ C_{22}H_{28}N_{2}O_{2} \\ C_{12}H_{6}CI_{4}O_{2}S \\ \end{array}$	Quinoxyfen Tebuconazole Fenamidone Kresoxim-methyl Flusilazole Myricetin Iprovalicarb Benalaxyl Fenarimol Tebufenpyrad Boscalid Thiophanat-methyl Tolyfluanid Tebufenozide Tetradifon (mono)	Flavanol Pesticides Pesticides Pesticides Pesticides Pesticides Pesticides Flavanol Pesticides
303.0135 303.0499 308.004 308.1524 312.1165 314.1387 316.1076 319.0448 321.2173 326.1751 331.0399 334.1681 343.0399 343.0529 346.9852 353.2224 354.8915 355.1024	$\begin{array}{c} C_{15}H_{10}O_{7} \\ C_{15}H_{8}CI_{2}FNO \\ C_{16}H_{22}CIN_{3}O \\ C_{17}H_{17}N_{3}OS \\ C_{18}H_{19}NO_{4} \\ C_{16}H_{15}F_{2}N_{3}Si \\ C_{15}H_{10}O_{8} \\ C_{18}H_{28}N_{2}O_{3} \\ C_{20}H_{23}NO_{3} \\ C_{17}H_{12}CI_{2}N_{2}O \\ C_{18}H_{24}CIN_{3}O \\ C_{18}H_{12}CI_{2}N_{2}O \\ C_{12}H_{14}N_{4}O_{4}S_{2} \\ C_{10}H_{13}CI_{2}FN_{2}O_{2}S_{2} \\ C_{22}H_{28}N_{2}O_{2} \\ C_{12}H_{6}CI_{4}O_{2}S \\ C_{16}H_{18}O_{9} \\ \end{array}$	Quercetin Quinoxyfen Tebuconazole Fenamidone Kresoxim-methyl Flusilazole Myricetin Iprovalicarb Benalaxyl Fenarimol Tebufenpyrad Boscalid Thiophanat-methyl Tolyfluanid Tebufenozide Tetradifon (mono) Chlorogenic acid	Flavanol Pesticides Pesticides Pesticides Pesticides Pesticides Pesticides Flavanol Pesticides
303.0135 303.0499 308.004 308.1524 312.1165 314.1387 316.1076 319.0448 321.2173 326.1751 331.0399 334.1681 343.0399 343.0529 346.9852 353.2224 354.8915 355.1024 356.8886 325.0521	$\begin{array}{c} C_{15}H_{10}O_{7} \\ C_{15}H_{8}CI_{2}FNO \\ C_{16}H_{22}CIN_{3}O \\ C_{17}H_{17}N_{3}OS \\ C_{18}H_{19}NO_{4} \\ C_{16}H_{15}F_{2}N_{3}Si \\ C_{15}H_{10}O_{8} \\ C_{18}H_{28}N_{2}O_{3} \\ C_{20}H_{23}NO_{3} \\ C_{17}H_{12}CI_{2}N_{2}O \\ C_{18}H_{24}CIN_{3}O \\ C_{18}H_{12}CI_{2}N_{2}O \\ C_{12}H_{14}N_{4}O_{4}S_{2} \\ C_{10}H_{13}CI_{2}FN_{2}O_{2}S_{2} \\ C_{22}H_{28}N_{2}O_{2} \\ C_{12}H_{6}CI_{4}O_{2}S \\ C_{12}H_{6}CI_{4}O_{2}S \\ C_{12}H_{6}CI_{4}O_{2}S \\ \end{array}$	Quercetin Quinoxyfen Tebuconazole Fenamidone Kresoxim-methyl Flusilazole Myricetin Iprovalicarb Benalaxyl Fenarimol Tebufenpyrad Boscalid Thiophanat-methyl Tolyfluanid Tebufenozide Tetradifon (mono) Chlorogenic acid Tetradifon (most abun)	Flavanol Pesticides Pesticides Pesticides Pesticides Pesticides Pesticides Flavanol Pesticides
303.0135 303.0499 308.004 308.1524 312.1165 314.1387 316.1076 319.0448 321.2173 326.1751 331.0399 334.1681 343.0399 343.0529 346.9852 353.2224 354.8915 355.1024 356.8886 325.0521 369.2173	$\begin{array}{c} C_{15}H_{10}O_{7} \\ C_{15}H_{8}CI_{2}FNO \\ C_{16}H_{22}CIN_{3}O \\ C_{17}H_{17}N_{3}OS \\ C_{18}H_{19}NO_{4} \\ C_{16}H_{15}F_{2}N_{3}Si \\ C_{15}H_{10}O_{8} \\ C_{18}H_{28}N_{2}O_{3} \\ C_{20}H_{23}NO_{3} \\ C_{17}H_{12}CI_{2}N_{2}O \\ C_{18}H_{24}CIN_{3}O \\ C_{18}H_{12}CI_{2}N_{2}O \\ C_{18}H_{14}N_{4}O_{4}S_{2} \\ C_{10}H_{13}CI_{2}FN_{2}O_{2}S_{2} \\ C_{22}H_{28}N_{2}O_{2} \\ C_{12}H_{6}CI_{4}O_{2}S \\ C_{12}H_{6}CI_{4}O_{2}S \\ C_{13}H_{13}CIN_{4}O_{2}S \\ C_{13}H_{13}CIN_{4}O_{2}S \\ \end{array}$	Quercetin Quinoxyfen Tebuconazole Fenamidone Kresoxim-methyl Flusilazole Myricetin Iprovalicarb Benalaxyl Fenarimol Tebufenpyrad Boscalid Thiophanat-methyl Tolyfluanid Tebufenozide Tetradifon (mono) Chlorogenic acid Tetradifon (most abun) Cyazofamid	Flavanol Pesticides Pesticides Pesticides Pesticides Pesticides Flavanol Pesticides
303.0135 303.0499 308.004 308.1524 312.1165 314.1387 316.1076 319.0448 321.2173 326.1751 331.0399 334.1681 343.0399 343.0529 346.9852 353.2224 354.8915 355.1024 369.2173 375.1339	$\begin{array}{c} C_{15}H_{10}O_{7} \\ C_{15}H_{8}CI_{2}FNO \\ C_{16}H_{22}CIN_{3}O \\ C_{17}H_{17}N_{3}OS \\ C_{18}H_{19}NO_{4} \\ C_{16}H_{15}F_{2}N_{3}Si \\ C_{15}H_{10}O_{8} \\ C_{18}H_{28}N_{2}O_{3} \\ C_{20}H_{23}NO_{3} \\ C_{17}H_{12}CI_{2}N_{2}O \\ C_{18}H_{24}CIN_{3}O \\ C_{18}H_{24}CIN_{3}O \\ C_{12}H_{14}N_{4}O_{4}S_{2} \\ C_{10}H_{13}CI_{2}FN_{2}O_{2}S_{2} \\ C_{22}H_{28}N_{2}O_{2} \\ C_{12}H_{6}CI_{4}O_{2}S \\ C_{12}H_{6}CI_{4}O_{2}S \\ C_{13}H_{13}CIN_{4}O_{2}S \\ C_{21}H_{28}N_{2}O_{3} \\ \end{array}$	Quercetin Quinoxyfen Tebuconazole Fenamidone Kresoxim-methyl Flusilazole Myricetin Iprovalicarb Benalaxyl Fenarimol Tebufenpyrad Boscalid Thiophanat-methyl Tolyfluanid Tebufenozide Tetradifon (mono) Chlorogenic acid Tetradifon (most abun) Cyazofamid Methoxyfenozide	Flavanol Pesticides Pesticides Pesticides Pesticides Pesticides Pesticides Flavanol Pesticides
303.0135 303.0499 308.004 308.1524 312.1165 314.1387 316.1076 319.0448 321.2173 326.1751 331.0399 343.0399 343.0529 346.9852 353.2224 354.8915 355.1024 369.2173 375.1339 388.1059	C <sub>15</sub> H <sub>10</sub> O <sub>7</sub> C <sub>15</sub> H <sub>8</sub> CI <sub>2</sub> FNO C <sub>16</sub> H <sub>22</sub> CIN <sub>3</sub> O C <sub>17</sub> H <sub>17</sub> N <sub>3</sub> OS C <sub>18</sub> H <sub>19</sub> NO <sub>4</sub> C <sub>16</sub> H <sub>15</sub> F <sub>2</sub> N <sub>3</sub> Si C <sub>15</sub> H <sub>10</sub> O <sub>8</sub> C <sub>18</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub> C <sub>20</sub> H <sub>23</sub> NO <sub>3</sub> C <sub>17</sub> H <sub>12</sub> CI <sub>2</sub> N <sub>2</sub> O C <sub>18</sub> H <sub>24</sub> CIN <sub>3</sub> O C <sub>18</sub> H <sub>24</sub> CIN <sub>3</sub> O C <sub>18</sub> H <sub>12</sub> CI <sub>2</sub> N <sub>2</sub> O C <sub>18</sub> H <sub>14</sub> N <sub>4</sub> O <sub>4</sub> S <sub>2</sub> C <sub>10</sub> H <sub>13</sub> CI <sub>2</sub> FN <sub>2</sub> O <sub>2</sub> S <sub>2</sub> C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>2</sub> C <sub>12</sub> H <sub>6</sub> CI <sub>4</sub> O <sub>2</sub> S C <sub>16</sub> H <sub>18</sub> O <sub>9</sub> C <sub>12</sub> H <sub>6</sub> CI <sub>4</sub> O <sub>2</sub> S C <sub>13</sub> H <sub>13</sub> CIN <sub>4</sub> O <sub>2</sub> S C <sub>21</sub> H <sub>26</sub> N <sub>2</sub> O <sub>3</sub> C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub> C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub>	Quercetin Quinoxyfen Tebuconazole Fenamidone Kresoxim-methyl Flusilazole Myricetin Iprovalicarb Benalaxyl Fenarimol Tebufenpyrad Boscalid Thiophanat-methyl Tolyfluanid Tebufenozide Tetradifon (mono) Chlorogenic acid Tetradifon (most abun) Cyazofamid Methoxyfenozide Famoxadone	Flavanol Pesticides Pesticides Pesticides Pesticides Pesticides Pesticides Flavanol Pesticides
303.0135 303.0499 308.004 308.1524 312.1165 314.1387 316.1076 319.0448 321.2173 326.1751 331.0399 334.1681 343.0399 3443.0529 346.9852 353.2224 354.8915 355.1024 356.8886 325.0521 369.2173 375.1339 388.1059 388.131	C <sub>15</sub> H <sub>10</sub> O <sub>7</sub> C <sub>15</sub> H <sub>8</sub> CI <sub>2</sub> FNO C <sub>16</sub> H <sub>22</sub> CIN <sub>3</sub> O C <sub>17</sub> H <sub>17</sub> N <sub>3</sub> OS C <sub>18</sub> H <sub>19</sub> NO <sub>4</sub> C <sub>16</sub> H <sub>15</sub> F <sub>2</sub> N <sub>3</sub> Si C <sub>15</sub> H <sub>10</sub> O <sub>8</sub> C <sub>18</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub> C <sub>20</sub> H <sub>23</sub> NO <sub>3</sub> C <sub>17</sub> H <sub>12</sub> CI <sub>2</sub> N <sub>2</sub> O C <sub>18</sub> H <sub>24</sub> CIN <sub>3</sub> O C <sub>18</sub> H <sub>24</sub> CIN <sub>3</sub> O C <sub>18</sub> H <sub>24</sub> CI <sub>2</sub> N <sub>2</sub> O C <sub>12</sub> H <sub>14</sub> N <sub>4</sub> O <sub>4</sub> S <sub>2</sub> C <sub>10</sub> H <sub>13</sub> CI <sub>2</sub> FN <sub>2</sub> O <sub>2</sub> S <sub>2</sub> C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>2</sub> C <sub>12</sub> H <sub>6</sub> CI <sub>4</sub> O <sub>2</sub> S C <sub>16</sub> H <sub>18</sub> O <sub>9</sub> C <sub>12</sub> H <sub>6</sub> CI <sub>4</sub> O <sub>2</sub> S C <sub>13</sub> H <sub>13</sub> CIN <sub>4</sub> O <sub>2</sub> S C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub> C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub> C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub> C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>4</sub> C <sub>19</sub> H <sub>18</sub> CIN <sub>3</sub> O <sub>4</sub>	Quinoxyfen Tebuconazole Fenamidone Kresoxim-methyl Flusilazole Myricetin Iprovalicarb Benalaxyl Fenarimol Tebufenpyrad Boscalid Thiophanat-methyl Tolyfluanid Tebufenozide Tetradifon (mono) Chlorogenic acid Tetradifon (most abun) Cyazofamid Methoxyfenozide Famoxadone Pyraclostrobin	Flavanol Pesticides Pesticides Pesticides Pesticides Pesticides Pesticides Flavanol Pesticides
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## SELECTED RESULTS

Wine (Area Counts)

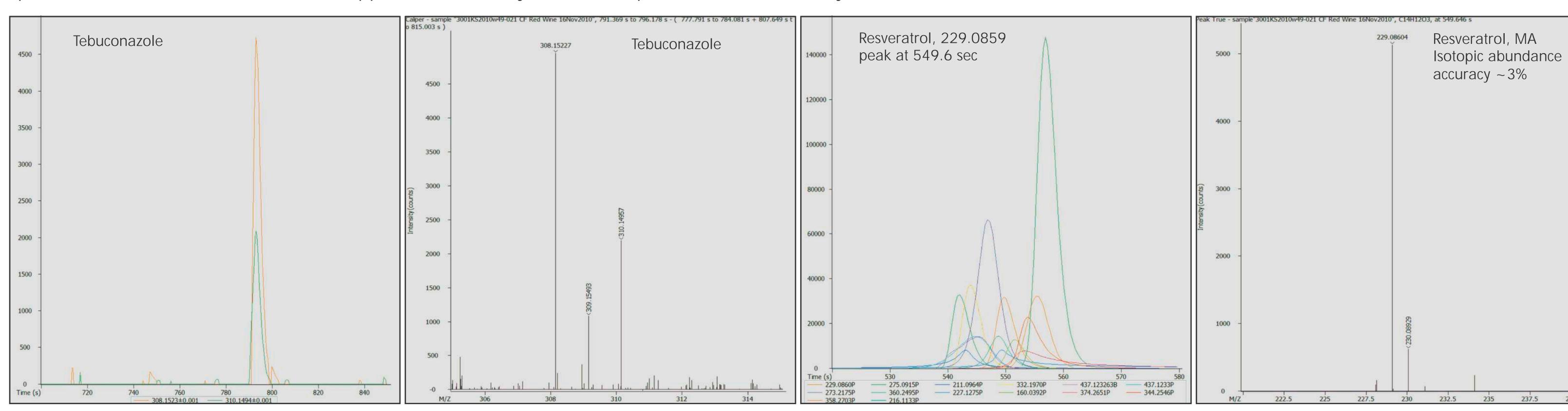
Grape Juice (Area Counts)

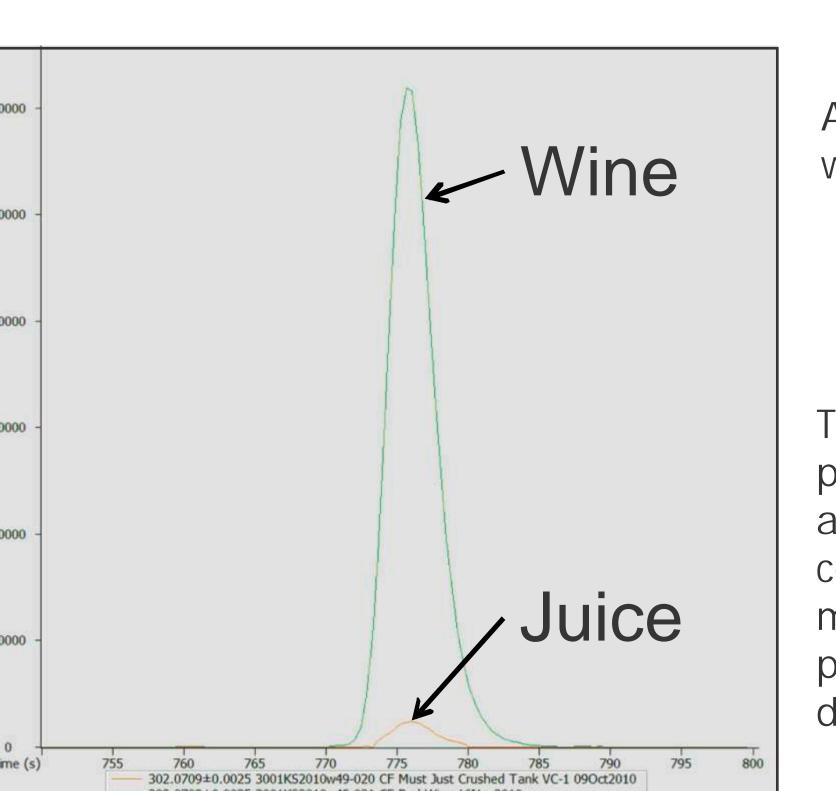
(M+H)+	Formula	Name	Class	Elution Time(s)	Cabernet Franc	Cabernet Franc Rose	Syrah	American Riesling	Vidal Blanc	Cabernet Franc Juice	Cab. Franc Rose Juice	Syrah Juice	Am Riesling Juice	Vidal Blanc Juice
165.0546	C <sub>9</sub> H <sub>8</sub> O <sub>3</sub>	Coumaric acid	Antioxidants	469	1.11E+06	4.78E+05	1.31E+06	n.d.	n.d.	tr.	n.d.	2.36E+07	1.63E+05	n.d.
169.0495	C <sub>8</sub> H <sub>8</sub> O <sub>4</sub>	Vanillic acid	Antioxidants	511	n.d.	2.12E+05	n.d.	n.d.	n.d.	tr.	n.d.	n.d.	n.d.	n.d.
199.0601	C <sub>9</sub> H <sub>10</sub> O <sub>5</sub>	Syringic acid	Antioxidants	466	3.20E+06	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	4.17E+06	n.d.	n.d.
200.1182	C <sub>12</sub> H <sub>13</sub> N <sub>3</sub>	Pyrimethanil	Pesticides*	634	1.71E+07	2.61E+07	2.65E+06	1.71E+06	3.04E+05	8.89E+05	8.71E+07	7.39E+04	1.73E+06	1.42E+06
229.0859	C <sub>14</sub> H <sub>12</sub> O <sub>3</sub>	Resveratrol	Antioxidants	550	3.19E+05	7.95E+05	8.71E+05	1.12E+06	5.88E+05	4.51E+05	n.d.	n.d.	n.d.	7.63E+04
287.055	C <sub>15</sub> H <sub>10</sub> O <sub>6</sub>	Kaempferol	Flavanol	636	3.41E+05	n.d.	8.69E+05	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
291.0863	C <sub>15</sub> H <sub>14</sub> O <sub>6</sub>	(epi) catechin	Flavanol	401	9.35E+06	3.79E+06	8.93E+06	n.d.	3.35E+06	7.70E+05	1.25E+07	2.26E+07	2.80E+06	4.84E+05
291.0863	C <sub>15</sub> H <sub>14</sub> O <sub>6</sub>	(epi) catechin	Flavanol	437	9.59E+06	5.42E+06	8.75E+06	6.82E+05	2.53E+06	5.70E+05	1.11E+07	1.86E+07	5.46E+05	3.57E+06
302.0709	C <sub>14</sub> H <sub>17</sub> Cl <sub>2</sub> NO <sub>2</sub>	Fenhexamid	Pesticides	775	6.15E+05	8.45E+05	7.18E+05	tr.	2.36E+05	n.d.	5.01E+05	5.01E+05	n.d.	n.d.
303.0499	C <sub>15</sub> H <sub>10</sub> O <sub>7</sub>	Quercetin	Flavanol	591	4.03E+07	3.41E+05	4.97E+07	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
308.1524	C <sub>16</sub> H <sub>22</sub> CIN <sub>30</sub>	Tebuconazole	Pesticides	792	n.d. (~4700 pk height)	~960 pk height	1.88E+05	tr.	1.16E+07	n.d.	n.d.	n.d.	n.d.	n.d.
319.0448	C <sub>15</sub> H <sub>10</sub> O <sub>8</sub>	Myricetin	Flavanol	540	4.58E+05	1.06E+07	1.24E+07	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
343.0399	C <sub>18</sub> H <sub>12</sub> CI <sub>2</sub> N <sub>20</sub>	Boscalid	Pesticides	762	1.42E+07	1.48E+07	1.24	1.47E+05	9.66E+05	n.d.	7.62E+05	9.50E+05	n.d.	n.d.
388.1059	C <sub>19</sub> H <sub>18</sub> CIN <sub>3</sub> O <sub>4</sub>	Pyraclostrobin	Pesticides	851	5.85E+05	6.94E+05	4.03E+05	n.d.	n.d.	n.d.	5.06E+05	n.d.	n.d.	n.d.
404.0895	C <sub>20</sub> H <sub>18</sub> CINO <sub>6</sub>	OTA (Ochratoxin A)	Mycotoxins	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
Total Molecular Features Detected with S/N > 50 across chromatogram			595	603	651	605	551	608	584	593	639	608		

Average of ~67 features in blanks run in the serie

#### DATA EXAMPLES

A low-level pesticide, Tebuconazole, was detected with 0.3 ppm mass accuracy and isotope abundance accuracy 2-3%. With the resveratrol, the peak is easily identified with the spectral deconvolution software at a 0.1 ppm mass accuracy and an isotopic abundance accuracy of ~3%.





An example of the apparent concentration of the pesticide, fenhexamid, in processed wine is shown at left for the Cabernet Franc wine/juice pair where the dominant peak is from the wine.

#### CONCLUSION

The Citius LC-HRT system provides a flexible research platform for screening of complex samples such as wine and fruit juice. The system provides for detection and identification of analytes over a wide dynamic range using the high mass resolution, high mass accuracy, accurate relative isotope abundance, and efficient spectral deconvolution inherent in the Citius. Analytical characterization of this type could prove useful to the wine industry to improve their processes and product consistency, and to provide a mechanism by which to monitor contaminants. Additional sample fractionation could result in deeper chemical reporting and management of the wine-making process. The results herein represent an example of the utility of TOFMS with high resolution and mass accuracy in combination with the dynamic range inherent in the Citius in the global analysis of complex mixtures such as fruit juice and wine.