Drug Residue Analysis by LC/MS methods

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Product Specialist
Agilent Technologies
Outline

🌟 General Drug Residue information

🌟 Veterinary drug residue Analysis by LC/MS QQQ and Q-TOF method

Agilent Technologies
Analytical Challenges in Drug Residues

1) ANALYTE DIVERSITY

- physico-chemical properties (polarity, pKa etc.)
- sample preparation (extraction, clean-up)
- analyte determination

LC-MS/MS is essential:

- universal, yet highly selective detection
- simultaneous quantitation and confirmation
- sensitive determination in complex matrices

- stability:
  - during analytical process and storage
  - in samples, standard solutions, extracts
Analytical challenges

2) MATRIX DIVERSITY

matrices:
- muscle
- kidney
- liver
- milk
- eggs
- urine
- blood

Considerations:
- matrix composition (lipids, proteins, carbohydrates, water, salts etc.)
- analyte-matrix interactions
- matrix coextractives
Determination of Tetracyclines residues in milk using Agilent 6410 LC/MS/MS
Introduction

◆ Tetracyclines are probably still the most frequently used antibiotics in animal husbandry

◆ Can lead to some disease, such as tetracycline stained teeth

◆ Compare with Classic HPLC/UV method, the LC/MS/MS can removal most of the background noise and get the excellent sensitivity in matrix
Issues for this analysis (1)

Sample preparation: even with all clean-up, there is still interference for OTC analysis in milk matrix

1. Stds in solvent

2. Stds in milk

3. Blank milk
Issues for this analysis (2)

There are total 3 pairs **isomers** in this analysis

1. Tetracycline and 4-Epitetracycline
2. Oxytetracycline and 4-epioxytetracycline
3. Chlortetracycline and 4-epichlortetracycline
Solution: LC/MS/MS Separations for the Isomers

QQQ Removes background interference and RRLC with good separation

- a. 4-epitetracycline
- b. Tetracycline
Sample Preparations

1. **Weight and harmonize**
   Weight 5 g milk sample (accurate to 0.01 g) into a 50 mL colorimetric tube, dissolved with 0.1 mol/L Na2EDTA-McIlvaine buffer solution and volume to 50 mL and vertex mixed for 1 min.

2. **Extraction**
   Ultrasonic extracted in ice water bath for 10 min, then transferred to 50mL polypropylene centrifugal tub, cooled down to 0°C~4°C, centrifuged at a rotate speed of 5000 r/min for 10 min (below 15°C)

3. **Purification**
   Accurately draw 10mL extract (equivalent to 1 g sample) and put it through the SPE cartridge—**SampliQ C18** at a speed of 1 drop/s. Then wash the cartridge with 5mL water and 5mL methanol + water in turn. Under a negative pressure below 2.0kPa, drain the cartridge for 5 min and collect the elute
Result in Real Sample-milk

- a. Milk matrix Blank
- b. TIC of 50ppb level in milk
- c. EIC of 50ppb level in milk
Linearity-in the milk

Methacycline

$R^2 = 0.9996$

Conc. 1ppb-1000ppb with 5uL injection
## Results

<table>
<thead>
<tr>
<th>Name</th>
<th>LOD in Milk by Agilent 6410 QQQ (pg on column)</th>
</tr>
</thead>
<tbody>
<tr>
<td>minocycline</td>
<td>16.3</td>
</tr>
<tr>
<td>4-epitetracycline</td>
<td>8.7</td>
</tr>
<tr>
<td>4-epioxytetracycline</td>
<td>12.8</td>
</tr>
<tr>
<td>tetracycline</td>
<td>10.2</td>
</tr>
<tr>
<td>oxytetracycline</td>
<td>8.6</td>
</tr>
<tr>
<td>demethylclocycline</td>
<td>8.1</td>
</tr>
<tr>
<td>4-epichlortetracycline</td>
<td>11.9</td>
</tr>
<tr>
<td>chlortetracycline</td>
<td>7.6</td>
</tr>
<tr>
<td>methacycline</td>
<td>12.3</td>
</tr>
<tr>
<td>doxycycline</td>
<td>11.2</td>
</tr>
</tbody>
</table>

**EU requirement:**
- Tetracycline in milk MRL 100ug/kg;

**US FDA requirement:**
- Tetracycline in milk MRL 300ug/kg

**China Gov Standard:**
- Tetracycline in milk: 50ug/kg

**Notes:** This is the calculation result at s/n=3 with injection 5uL
## Repeatability

<table>
<thead>
<tr>
<th>Name</th>
<th>R² in milk</th>
<th>RSD of Signal response at 50ppb (n=6)</th>
<th>RSD of Ion ration (n=6)</th>
</tr>
</thead>
<tbody>
<tr>
<td>minocycline</td>
<td>0.990</td>
<td>4.9</td>
<td>2.1</td>
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<tr>
<td>4-epitetracycline</td>
<td>0.994</td>
<td>3.8</td>
<td>1.5</td>
</tr>
<tr>
<td>4-epioxytetracycline</td>
<td>0.996</td>
<td>5.4</td>
<td>1.3</td>
</tr>
<tr>
<td>tetracycline</td>
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<td>2.5</td>
<td>1.2</td>
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<tr>
<td>oxytetracycline</td>
<td>0.993</td>
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<td>1.6</td>
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<td>demethylclocycline</td>
<td>0.987</td>
<td>2.0</td>
<td>3.1</td>
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<tr>
<td>4-epichlortetracycline</td>
<td>0.994</td>
<td>5.5</td>
<td>5.4</td>
</tr>
<tr>
<td>chlortetracycline</td>
<td>0.994</td>
<td>4.5</td>
<td>1.5</td>
</tr>
<tr>
<td>methacycline</td>
<td>0.999</td>
<td>1.0</td>
<td>1.9</td>
</tr>
<tr>
<td>doxycycline</td>
<td>0.995</td>
<td>3.6</td>
<td>6.7</td>
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</tbody>
</table>
Conclusions

• Easy of method development and set-up
• High sensitivity even in food matrix
• Wide dynamic range for the quantification
• Qualifier ion and quantifier ion and their ration can double confirm and identify compound in the matrix
• Easily to meet the world wide regulation
Conclusions

- Agilent LC-MS/MS provides the means to develop faster and easier methods to detect ultratrace levels of veterinary drug and other polar chemicals of interest in foods
  - Easy of method development and set-up
  - High sensitivity even in food matrix
  - Wide dynamic range for the quantification
  - Qualifier ion and quantifier ion and their ration can double confirm and identify compound in the matrix
  - Easily to meet the world wide regulation

- Using Agilent NEW SPE product can make sample preparation easier and can get excellent result
Screening and Confirming Antibiotic in Chicken and Milk Extract using Agilent 1200 RRLC and 6520 QTOF MS
Workflow Solution

Screening

• Data acquired under full scan mode as profile format
• Data processed using
  – Find by MEF and Mass profiler

Confirming

• Develop Target MS/MS method for analyzing all compounds found in spiked sample
• Data processed using ‘find compound by target MS/MS’
## Screening and confirming antibiotic in chicken

<table>
<thead>
<tr>
<th></th>
<th>5 ppb (10 pg on column)</th>
<th>10 ppb (20 pg on column)</th>
<th>20 ppb (40 pg on column)</th>
<th>50 ppb (100 pg on column)</th>
<th>100 ppb (200 pg on column)</th>
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<td><strong>Target compound hits</strong></td>
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<td>8</td>
<td>8</td>
<td>8</td>
<td>8</td>
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<tr>
<td><strong>Hit rate</strong></td>
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<td>100%</td>
<td>100%</td>
<td>100%</td>
<td>100%</td>
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<tr>
<td><strong>Fault positive result</strong></td>
<td>3</td>
<td>20</td>
<td>16</td>
<td>16</td>
<td>6</td>
</tr>
</tbody>
</table>
sample at 5ppb concentration level compared with matrix blank
4-Epitetracycline  Rt=3.5 min
Conclusions

Q-TOF is the good tool for Targeted and Unknown Screening.

- Accurate Mass provides added compound selectivity
- Always full spectral data using the TOF mode
- Unlimited number of compounds can be screened (search exact mass compound database for identification)
- Sensitivity is the same regardless of number of compounds screened
- Target MS/MS of Q-TOF assists compound confirmation
Screening and confirming Mycotoxin in wheat extract using Agilent 1200 RRLC and 6520 QTOF MS
Technical Challenges in this analysis

Looking for a needle in the haystacks??????

Agilent 6520 Q-TOF solution provide the excellent result for such kind of analysis
### Result obtained by MFE

<table>
<thead>
<tr>
<th></th>
<th>5 ppb</th>
<th>10 ppb</th>
<th>20 ppb</th>
<th>50 ppb</th>
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<td>10</td>
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<td>4</td>
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<td><strong>Hit rate</strong></td>
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<td>80%</td>
<td>100%</td>
<td>100%</td>
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<td>7</td>
<td>5</td>
<td>6</td>
<td>11</td>
<td>5</td>
</tr>
</tbody>
</table>
Parameters setting - MFE

**Extraction**
- **Target data type**: Small molecules (chromatographic)
- **Input data range**
  - Restrict retention time
  - Restrict m/z
- **Peak filters**
  - Use peaks with signal-to-noise
    - Profile spectra only
    - Signal-to-noise ratio >= 5.0
  - Use peaks with height
    - Profile and centroid spectra
    - Height >= 100 counts
- **Height**
  - Relative height
  - Absolute height
    - Height >= 100 counts
  - Limit to the largest
    - Number of compounds
- **Compound location**
  - Restrict retention times
- **Charge states**
  - Restrict charge states
- **MHD file filtering**
  - Apply all filters to MHD file
  - Do not filter MHD file

**Ion Species**
- **Positive ions**
  - H
  - Na
  - K
  - NH4
- **Negative ions**
  - Cl
  - Br
  - HCOO
  - CH3COO
  - CF3COO
- **Neutral losses**
  - H2O
  - H3PO4

**Charge State**
- **Neutral losses**
  - H2O
  - H3PO4

**Compound Filters**
- **Mass filters**
  - Filter mass list
    - Mass limit: 5.00 ppm
    - Exclude these masses
  - Source of masses
    - These masses

**Mass Defect**
- Mass defect

*Agilent Technologies*
Spiked target compounds at 5 ppb concentration level

<table>
<thead>
<tr>
<th>Name</th>
<th>File</th>
<th>Cod</th>
<th>RT</th>
<th>Mass</th>
<th>Formula (DB)</th>
<th>Diff (DB, ppm)</th>
<th>Score (DB)</th>
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<th>Height</th>
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<tr>
<td>ochratoxin A</td>
<td>mycotoxin-prof...</td>
<td>1165</td>
<td>12.247</td>
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<td>C20 H18 Cl N O6</td>
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<td>fumonisin B1</td>
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<td>1935</td>
<td>14.15</td>
<td>408.1719</td>
<td>C22 H29 Cl O5</td>
<td>-3.75</td>
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<td>705.3964</td>
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<td>flunonicoil amine</td>
<td>mycotoxin-prof...</td>
<td>240</td>
<td>0.63</td>
<td>374.0241</td>
<td>C12 H17 C2 F...</td>
<td>7.87</td>
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<td>Anoxicillin</td>
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<td>499</td>
<td>0.728</td>
<td>365.1014</td>
<td>C16 H19 N3 O5 S</td>
<td>8.47</td>
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<tr>
<td>minocycline</td>
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<td>114</td>
<td>0.572</td>
<td>457.1809</td>
<td>C23 H27 N O7</td>
<td>8.3</td>
<td>45.88</td>
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<td>334</td>
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</table>

3 out of 10 compounds had hit from database search
<table>
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<tr>
<th></th>
<th>5 ppb</th>
<th>10 ppb</th>
<th>20 ppb</th>
<th>50 ppb</th>
<th>100 ppb</th>
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<tr>
<td><strong>Total hits</strong></td>
<td>19</td>
<td>17</td>
<td>16</td>
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<td>12</td>
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<td><strong>Target compound hits</strong></td>
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<td>5</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td><strong>Hit rate</strong></td>
<td>100%</td>
<td>100%</td>
<td>100%</td>
<td>100%</td>
<td>100%</td>
</tr>
<tr>
<td><strong>Fault positive result</strong></td>
<td>14</td>
<td>12</td>
<td>11</td>
<td>9</td>
<td>7</td>
</tr>
</tbody>
</table>
Parameters setting- ’find by formula’

**Formula Source**
- These formulas: C20H13NO5Cl
  (type a comma-separated list of formulas, e.g., "C6H6, CH4")
- Database:
  D:\MassHunter\databases\Metlin_veterinary-new.mnl
- Worklist

**Source of formulas to confirm**

**Database values to match**
- Mass
- Mass and retention time (retention time optional)
- Mass and retention time (retention time required)

**Formula Matching**
- Match tolerance
  - Masses: +/- 5.00 ppm
  - Retention times: +/- 0.500 minutes

**Expansion of values for chromatogram extraction**
- Possible m/z: Symmetric (ppm) +/- 10.0
- Expected retention time: +/- 1.50 minutes

**EIC Integration**
- EIC Peak Filters
  - Integrator selection
    - General MS Integrator

**Options**
- Detector
  - Point sampling: 3
  - Smoothing
  - Stop threshold: 0.0
- Filtering: 5 point
  - Peak location: Top
- Baseline allocation
  - Baseline reset: 5
  - If either edge: 100%
  - Tangent skim else drop
Spiked target compounds at 5 ppb concentration level

<table>
<thead>
<tr>
<th>Name</th>
<th>File</th>
<th>Cpd</th>
<th>RT</th>
<th>Mass</th>
<th>Formula (DB)</th>
<th>Diff (DB, ppm)</th>
<th>Score (DB)</th>
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<tbody>
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<td>lumonian B2</td>
<td>mycotoxin-profil...</td>
<td>208</td>
<td>9.376</td>
<td>705.3948</td>
<td>C34 H59 N O14</td>
<td>-1.78</td>
<td>90.25</td>
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<td>170</td>
<td>12.231</td>
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<td>C20 H18 Cl N O6</td>
<td>1.36</td>
<td>88.51</td>
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<td>8.751</td>
<td>239.1513</td>
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<td>Zeranol</td>
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<td>C18 H26 O5</td>
<td>1.09</td>
<td>79.51</td>
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<td>zearelanone</td>
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<td>102</td>
<td>14.115</td>
<td>320.1614</td>
<td>C18 H24 O5</td>
<td>3.08</td>
<td>74.99</td>
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<td>Flumethasone acetate</td>
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<td>190</td>
<td>9.212</td>
<td>452.2003</td>
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<td>0.29</td>
<td>74.15</td>
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<td>14.181</td>
<td>259.158</td>
<td>C16 H21 N O2</td>
<td>-3.06</td>
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<td>99</td>
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<td>Triamcinolone acetonide</td>
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<td>185</td>
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<td>434.2105</td>
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<td>-0.12</td>
<td>60.1</td>
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<td>Trenbolone</td>
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<td>55</td>
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<td>sulfasalazine</td>
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<td>300.0673</td>
<td>C14 H12 N4 O2 S</td>
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<td>Chloramphenicol(Chloramphenicol)</td>
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<td>103</td>
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<td>322.013</td>
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<td>46.2</td>
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<td>Ofloxacin</td>
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<td>145</td>
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<td>C18 H20 F N3 O4</td>
<td>-2.12</td>
<td>45.93</td>
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<td>Albendazole-Sulfone</td>
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<td>4.67</td>
<td>45.43</td>
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<td>24</td>
<td>10.363</td>
<td>224.0533</td>
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<td>45</td>
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Results obtained by Mass Profiler and Metlin

<table>
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<tr>
<th></th>
<th>5 ppb</th>
<th>10 ppb</th>
<th>20 ppb</th>
<th>50 ppb</th>
<th>100 ppb</th>
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<td>Total hits</td>
<td>11</td>
<td>9</td>
<td>8</td>
<td>8</td>
<td>11</td>
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<tr>
<td>Target compound hits</td>
<td><strong>3</strong></td>
<td><strong>4</strong></td>
<td><strong>4</strong></td>
<td><strong>5</strong></td>
<td><strong>5</strong></td>
</tr>
</tbody>
</table>
sample at 5ppb concentration level compared with matrix blank

Features distribution map, total 1669 features were found in sample at 5 ppb concentration level
The Metlin database search result demonstrates that 11 compounds have hit from database search, and 4 out of 11 compounds have hit target compounds.

**Batch Summary Results:** 10 hits (11 total hits, 9 single matches, 1669 submitted)

<table>
<thead>
<tr>
<th>Mass Submitted</th>
<th>Delta Mass (ppm)</th>
<th>RT Submitted</th>
<th>Delta RT</th>
<th>Name</th>
<th>Formula</th>
<th>Mass</th>
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<tbody>
<tr>
<td>300.20690</td>
<td>6.76</td>
<td>14.538</td>
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<td>methandrostenolone</td>
<td>C20H28O2</td>
<td>300.20893</td>
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<tr>
<td>434.20770</td>
<td>6.37</td>
<td>0.706</td>
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<td>Triamcinolone acetonide</td>
<td>C24H31F06</td>
<td>434.21047</td>
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<td>721.39740</td>
<td>1.48</td>
<td>7.996</td>
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<td>fumonisin B1</td>
<td>C34H59N1O15</td>
<td>721.38847</td>
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<tr>
<td>317.27000</td>
<td>-0.43</td>
<td>14.700</td>
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<td>amorolfine</td>
<td>C21H35N0</td>
<td>317.27186</td>
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<tr>
<td>408.17160</td>
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<td>beclomethasone</td>
<td>C22H29ClO5</td>
<td>408.17035</td>
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<tr>
<td>392.20120</td>
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<td>0.711</td>
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<td>Betamethasone</td>
<td>C22H29F05</td>
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<td>Zearal</td>
<td>C18H26O5</td>
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</tr>
</tbody>
</table>
Conclusions

Q-TOF is the good tool for Targeted and Unknown Screening.

- Accurate Mass provides added compound selectivity
- Always full spectral data using the TOF mode
- Unlimited number of compounds can be screened (search exact mass compound database for identification)
- Target MS/MS of Q-TOF assists compound confirmation