High Resolution LC-QTOF MS for the Screening of Unknown Contaminants in Biological and Environmental Samples

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Biomonitoring Branch, ECL
Department of Toxic Substance Control
9/28/16
Why QTOF Screening? Beyond the targeted analytes list
Agilent 6550 LC QTOF

- Mass accuracy: sub ppm level
- High resolution
- No loss of data across entire monitored m/z range (100-1700, “small molecule”)
Presentation Outline

• System and Projects Overview
• Target Suspect Screening -> Non-target Suspect Screening -> Semi-Unknown approach
• Projects Summary (biological and environmental samples)
  1. SFO waste water screening
  2. Cat serum screening
  3. Foam Project
1. Target Suspect Screening: Samples with interested Targeted Chemical Family
   FBF (find by formula) algorithm

2. Non Target Suspect Screening: not limited to one particularly family but expand to broader non target contaminants
   MFE (molecular feature extraction) algorithm

3. Semi-Unknown Approach: beyond current databases
Projects Overview

• **SFO waste water**: historical usage and current annual testing of AFFF (aqueous fire fighting foam) at SFO result in high concentration of PFASs in waste water. What are those precursors/intermediates in the WW in the treatment plants before discharge to bay? **Target Suspect Screening**

• **Cat serum exposome screening**: a pilot project to set up biomonitoring/serum sample method on the QTOF. Convenient samples of 5 HT cats and 5 Normal cats serum. compounds profiles comparison between HT and Normal cats. **Non Target Suspect + Semi Unknown**

• **Participate in the safer consumer product projects (SB-1019 labeling)**: help confirm if there is no presence of OPFRs, as well as expand identification of other FRs present in fabric/foams: in the process of summarize into a standard method. **Target Suspect Screening**
Library

1. organo-phosphate flame retardants (OPFR) library: 92
2. Expanded PFAS library: 244
3. In House LCMS library (using consumer product chemicals index, combine with our in-house chemicals and up to date literatures): ~2500
4. EPA Tox21 library (DSSTox_ToxCastRelease_20151019): ~9000
5. EOA library (Environmental organic acids, Collaboration Project with UCSF): 744

SFO Waste Water Screening: Target Suspect Screening

- A spin-off project from our LC-MS/MS methods of PFAS analysis
Timeline of Sampling (2015)

- 11/19: First AFFF Addition
- 11/25: 12/1: More AFFF
- 12/2: 12/3: End of AFFF
- 12/6: 12/9: 12/14: 12/15

Sample collected
- Analyzed by LC-MS/MS for PFAS Suite
- Analyzed by TOP Assay
- Analyzed by LC-QTOF-MS

Erika Houtz et al, 2016 ACS presentation, San Diego
Total PFAS level (TOP assay) much higher than total concentration of targeted PFAS measured in the waste water.
workflow

Full Scan TIC, triplicate data set

Inspect Data Quality, RT shift, peak intensity

FBF (Find By Formula using appropriate parameters), search against PFAS library

MPP for compounds
Grouping and Alignment, and blank substraction

Recursive Qual Analysis
1. Generate Compound list
2. Inspect Chromatography
3. Inspect Mass spectrum
4. review overall score

Further Identification and confirmation
1. Literature search
2. Standard comparison
3. MS/MS spectra
A database was compiled, which contained the masses and elemental formulas for all potential AFFF fluorochemicals identified in patents.

105 compounds identified in AFFF samples: C₃-C₁₅
Accurate mass

Well defined Chromatography Peak

Isotopic pattern match
Katie C. Harding-Marjanovic et al., Environ. Sci. Technol. 2015, 49, 7666–7674
SFO WW Screening

• Expand the analytes list beyond the original LC-MS/MS method: found precursors, intermediates, and new replacement PFASs: ADONA, Ether-PFHxS, Ketone-PFOS
• Help confirmation of the sources and transformation pathways
• Working on Compare WW profiles from different sources: MPP analysis
Previously, we have used LC-MS/MS serum method to analyze 12 PFAS compounds in cat serum samples.

- Pilot project for **biological sample** QTOF screening
Temporal Changes of PBDE Levels in California House Cats and a Link to Cat Hyperthyroidism

Weihong Guo†, Stephen Gardner‡, Simon Yen§, Myrto Petreas†, and June-Soo Park†
† California Department of Toxic Substances Control, California Environmental Protection Agency, 700 Heinz Avenue, Berkeley, California 94710, United States
‡ VCA Albany Animal Hospital, 1550 Solano Avenue, Albany, California 94707, United States
§ Campus Veterinary Clinic, 1607 M.L.K. Jr Way, Berkeley, California 94709, United States
Questions Asked For This Study

1. Exposome of Cat Serum: Non Target Suspect Screening: Beyond the 12 common PFCAs;

High production volume (HPV) chemicals, pharmaceuticals, pesticides, poly and perfluoroalkyl substances (PFAS) and flame retardants

2. Are there detectable profile differences between the control and case groups?
Serum Prep: a simple protein precipitation method

- Vortex
- MeOH
- Centrifuge
- Evaporation
- Reconstitution and instrument analysis
the MPP (Mass Profiler Professional) non targeted workflow

- Full Scan TIC, triplicate injections
- MFE (Molecular Feature Extraction) with appropriate parameters
- Export to MPP, Grouping and Alignment: Features aligned across all data sets
- Apply Quality Control Filters, Blank subtraction, Recursive analysis

Peak filter
- Mass tolerance
- RT tolerance
- Ion species
Export for Identification:
- exact mass, isotope pattern, retention time
1. Search against databases
2. Unknowns: elemental formula generation

Profiles Comparison MPP
1. Group as control and case
2. Comparison using volcanic plot, p <0.05, fold >2

Identify features that are up or down regulated between case and control groups

Further Identification and confirmation
1. Search Chemspider/Pubmed and/or Merck Index (search by formula, by accurate mass)
2. MS/MS spectra
Cat Exposome: All 10 samples

Feature: Mass@RT

~1300 after alignment

Cpd 1343: C10 H20 O2: -ESI EIC(171.1391, 217.1445, 231.1602) Scan Fract=375.0V cat serum N_neg_05_02.d
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<thead>
<tr>
<th>Cpd</th>
<th>Label</th>
<th>Name</th>
<th>RT</th>
<th>Formula</th>
<th>Score</th>
<th>Mass</th>
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<td>benzoic acid</td>
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<td>Cpd 4</td>
<td>allyl caproate</td>
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<td>C9 H16 O2</td>
<td>99.03</td>
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<td>Cpd 1</td>
<td>1-octen-3-ol</td>
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<td>C8 H16 O</td>
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<td>771</td>
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<td>ID 0270 - from: Env. Science Technol., 2013, 47 (10),</td>
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<td>97.69</td>
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<td>423</td>
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<td>734</td>
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<td>1,2-[2,2-bis(2-methylpropyl)ethyl]hexane</td>
<td>5.618</td>
<td>C8 H5 F13 O3 S</td>
<td>97.04</td>
<td>427.9748</td>
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</tbody>
</table>
Present in only one sample
HT vs. Normal: Profiles comparison

Venn diagram, HT vs. Normal
Volcano plot: Up vs Down Regulation

5 vs 5: very limited sample size

Down regulated entities

Up regulated entities
### Profile comparison: HT vs. Normal

ID Browser Up regulated, Score > 80

<table>
<thead>
<tr>
<th>Name</th>
<th>Formula</th>
<th>Mass</th>
<th>RT</th>
<th>Score</th>
<th>comment</th>
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</thead>
<tbody>
<tr>
<td>Duloxetine</td>
<td>C18 H19 N O S</td>
<td>343.1241</td>
<td>5.617</td>
<td>96.76</td>
<td>depression drug</td>
</tr>
<tr>
<td>PFOSA</td>
<td>C8 H2 F17 N O2 S</td>
<td>498.953</td>
<td>6.568</td>
<td>96.73</td>
<td>PFAS</td>
</tr>
<tr>
<td>PFOSAA</td>
<td>C10 H4 F17 N O4 S</td>
<td>556.9582</td>
<td>6.236</td>
<td>95.59</td>
<td>PFAS</td>
</tr>
<tr>
<td>Catechol</td>
<td>C6 H6 O2</td>
<td>110.0368</td>
<td>0.905</td>
<td>87.47</td>
<td>phenol/pesticide</td>
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<tr>
<td>L-leucine</td>
<td>C6 H13 N O2</td>
<td>131.0947</td>
<td>0.619</td>
<td>86.86</td>
<td>dietary supplement</td>
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<tr>
<td>acetaminophen</td>
<td>C8 H9 N O2</td>
<td>151.0634</td>
<td>1.458</td>
<td>86.75</td>
<td>pharmaceutical</td>
</tr>
<tr>
<td>texanol</td>
<td>C12 H24 O3</td>
<td>216.1722</td>
<td>5.738</td>
<td>86.44</td>
<td>coalescent for latex paints</td>
</tr>
<tr>
<td>myristic acid</td>
<td>C14 H28 O2</td>
<td>228.2093</td>
<td>7.208</td>
<td>85.83</td>
<td>common fatty acid</td>
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<tr>
<td>acetophenone</td>
<td>C8 H8 O</td>
<td>120.0569</td>
<td>5.286</td>
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<td>common fragrant ketone used in fragance</td>
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<tr>
<td>(S)-hydroprene</td>
<td>C17 H30 O2</td>
<td>266.2239</td>
<td>7.274</td>
<td>85.37</td>
<td>insecticide</td>
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<tr>
<td>dodecyl methacrylate</td>
<td>C16 H30 O2</td>
<td>254.2236</td>
<td>7.644</td>
<td>82.19</td>
<td>an ester that might be used in PCP</td>
</tr>
</tbody>
</table>
### Identification with (LC-HR)MS/MS – Confidence?

Proposed levels for MS and MS/MS data

<table>
<thead>
<tr>
<th>Example</th>
<th>Identification confidence</th>
<th>Minimum data requirements</th>
</tr>
</thead>
</table>
| ![Molecule](image1.png) | **Level 1: Confirmed structure**  
  by reference standard | MS, MS\(^2\), RT, Reference Std.               |
| ![Molecule](image2.png) | **Level 2: Probable structure**  
  a) by library spectrum match  
  b) by diagnostic evidence | MS, MS\(^2\), Library MS\(^2\)  
 MS, MS\(^2\), Exp. data |
| ![Molecule](image3.png) | **Level 3: Tentative candidate(s)**  
  structure, substituent, class | MS, MS\(^2\), Exp. data                      |
| ![Molecule](image4.png) | **Level 4: Unequivocal molecular formula** | MS isotope/adduct                             |
| ![Molecule](image5.png) | **Level 5: Exact mass of interest** | MS                                            |

---

# Profile comparison: HT vs. Normal

ID Browser Up regulated, Score > 80

<table>
<thead>
<tr>
<th>Name</th>
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<tbody>
<tr>
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<td>Catechol</td>
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<td>phenol/pesticide</td>
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<td>131.0947</td>
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<td>151.0634</td>
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<td>254.2236</td>
<td>7.644</td>
<td>82.19</td>
<td>an ester that might be used in PCP</td>
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</tbody>
</table>
Tentatively identified compounds, Down regulated

<table>
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<tr>
<th>Name</th>
<th>Formula</th>
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<tr>
<td>Lufenuron</td>
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<td>(+)-isostearic acid</td>
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</tbody>
</table>

**Database match**

**Molecular Formula Generation**
Semi-Unknowns: Those that have No Database match

20 Formula Generated

| TRUE | C15 H24 N2 O3 P S | 97.8 343.1243 | 343.1245 0.59 0.59 0.2 5.617 |
| FALSE | C19 H21 N O3 S | 97.01 343.1243 | 343.1242 -0.14 0.14 -0.05 5.617 |

2570 Formula match in ChemSpider
Case Study #2

Halogen Containing Features

18 formulas $\rightarrow$ C14H10Cl2N2O2S

352 hits, ChemSpider
Case Study #3

Compounds: C10 H7 Cl3 F6 N2 O2; 5.860 min - FBF Spectrum (5.860 min)

Counts vs. Mass-to-Charge (m/z): x10^5

- 404.9403 (M-H)-
- 405.9423 (M-H)-
- 406.9375 (M-H)-
- 407.9393 (M-H)-
- 408.9338 (M-H)-
**C10H13BrF2N2O4S2**

**Found 3 results**

Search term: C10H13BrF2N2O4S2 (Found by molecular formula)

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<th>Structure</th>
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<th>Molecular Weight</th>
<th># of Data Sources</th>
<th># of References</th>
<th># of PubMed</th>
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</table>
USING MASS SEARCH

Merck Index: search by formula mass, low resolution

EPA CompTox Dashboard: Search by monoisotopic Mass, high resolution
Case Study #3

EPA comptox dashboard, mass search

46 hit

Searched by Mass and single component chemicals: Found 46 results for '405.9483 ± 0.035 amu'.

<table>
<thead>
<tr>
<th>Structure</th>
<th>Preferred Name</th>
<th>CAS-RN</th>
<th>QC Level</th>
<th>Number of Sources</th>
<th>Monoisotopic Mass</th>
<th>Mass Difference</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>Chlorfenapy</td>
<td>122453-73-0</td>
<td>DSSTox Low</td>
<td>24</td>
<td>405.969538</td>
<td>0.0212</td>
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<td></td>
<td>Diclazuril</td>
<td>101831-37-2</td>
<td>DSSTox Low</td>
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<td>405.979109</td>
<td>0.0308</td>
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EPA comptox dashboard, mass search

405.9483 ± 0.0035

Case Study #3

Trisulfide, bis[(4-methylphenyl)sulfonyl]

5692-44-4 | DTXSID10399230

Searched by Mass and single component chemicals: Found 1 result for '405.9483 ± 0.0035 amu'.

Intrinsic Properties

Molecular Formula: C14H14O4S5
Average Mass: 486.56 g/mol
Monoisotopic Mass: 405.949565 g/mol

Structural Identifiers

Record Information

Summary

Octanol-Water Partition Coefficient (LogP)
Water Solubility
Melting Point

Download as: CSV Excel SDF

<table>
<thead>
<tr>
<th>Property</th>
<th>Average (Exp.)</th>
<th>Median (Exp.)</th>
<th>Range (Exp.)</th>
<th>Average (Pred.)</th>
<th>Median (Pred.)</th>
<th>Range (Pred.)</th>
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<td>Octanol-Water Partition Coefficient (LogP)</td>
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<td>2.00</td>
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<td>Water Solubility</td>
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<td>18%</td>
<td>18% (1)</td>
<td>18% (1)</td>
<td>18%</td>
<td>-</td>
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</table>
Cat Exposome Screening Summary

- Established method for biological sample prep and screening. The biological exposome includes: various PFASs, PCPs, pesticides, pharmaceuticals, FRs
- Exploratory project on profiles comparison: procedures, criteria's
- SOP in process
What’s Next?

Slide from Jon Sobus presentation, US EPA
Standard Protocols, Suspect Screening

- Flame Retardants
- EOA/Exposome/Metabolimics
- Expanded PFAS
- Identification/Confirmation of new emerging contaminants.
  Develop new methods for Targeted/Quantification Analysis

Sample

Products (eg. Foam)

Serum

Waste water
Acknowledgements

B2 Group
HEMS Group
Dr. Steve Garner, Albany Animal Hospital, Albany, California, USA
William Zolan, Supervising Chemist, Mel Leong Treatment Plant
Dr. Bruce Labelle, ECL Chief
Diclazuril is used in cats to treat Isospora species.
Venn diagram

Entity List 1: E-blank
150 entities

Entity List 2: IN-blank
312 entities

Entity List 3: Mix-blank
267 entities
Targeted vs. non targeted SFO WW
MPP Data processing: non targeted workflow, recursive analysis.
Profile plots, 131 features: 76 up regulated, 55 down regulated
System Overview: Analysis method

HPLC system: Agilent UPLC 1290

- Agilent extended C18 column, 1.8 um, 2.1X50 mm
- Electrospray Ionization (ESI), negative/positive ion polarity
  full scan (m/z 100-1700)
- Two sets of Gradients for positive/negative ionization
- System Calibration before each run using Agilent Tuning mix
  (ESI-L Low Concentration Tuning Mix)
- References used during the sample run