Overview

- Staff Changes
- Methods Updates
- Projects: Ongoing and Pending
- Future Work
Staff Changes

CDC Grant positions
• EHL analysts: reduced from 5 to 2
• Core lab staff: reduced from 3 to 0

State positions: Two vacancies
• Replacing Dr. Simon Ip
• Limited-term (2-yr) position

Challenges in managing core tasks
• Sample management
• LIMS
• QA/QC
Methods Updates

- **Organophosphate (OP) Flame Retardants**
  MS/MS detection method developed; HPLC separation method in progress

- **Bisphenol A Analogs**
  Method developed and under validation

- **“Unknown” Screening**
  Toxic Chemical Finder (TCF) database developed; application is being testing against known compounds
<table>
<thead>
<tr>
<th>OP Flame Retardants Method</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Bis(1,3-dichloro-2-propyl) phosphate (BDCPP)</strong></td>
</tr>
<tr>
<td>![Bis(1,3-dichloro-2-propyl) phosphate (BDCPP)]</td>
</tr>
<tr>
<td><strong>Bis(2-chloroethyl) phosphate (BCEP)</strong></td>
</tr>
<tr>
<td>![Bis(2-chloroethyl) phosphate (BCEP)]</td>
</tr>
<tr>
<td><strong>Bis(2-chloroisopropyl) phosphate (BCPP)</strong></td>
</tr>
<tr>
<td>![Bis(2-chloroisopropyl) phosphate (BCPP)]</td>
</tr>
<tr>
<td><strong>Diphenyl phosphate (DPP)</strong></td>
</tr>
<tr>
<td>![Diphenyl phosphate (DPP)]</td>
</tr>
</tbody>
</table>
BPA Analogs*

**BPA**

**BPB**

**BPS**

**BPB**

**BPAF**

**BPF**

*p,p’-Bisphenols*
# Method Validation

<table>
<thead>
<tr>
<th></th>
<th>Linear range (ppb)</th>
<th>QC-Low-level</th>
<th>QC-High-level</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>0.5 ppb (n=9)</td>
<td>5 ppb (n=9)</td>
</tr>
<tr>
<td>BPS</td>
<td>0.1-50 (R²=0.967)</td>
<td>Precision (RSD) 6%</td>
<td>Accuracy (Recovery) 86%</td>
</tr>
<tr>
<td>BPB</td>
<td>0.1-100 (R²=0.982)</td>
<td>11%</td>
<td>94%</td>
</tr>
<tr>
<td>BPAF</td>
<td>0.1-8 (R²=0.996)</td>
<td>12%</td>
<td>86%</td>
</tr>
<tr>
<td>BPF</td>
<td>0.1-100 (R²=0.999)</td>
<td>6%</td>
<td>108%</td>
</tr>
</tbody>
</table>
Recently approved $250K upgrade of our *Exactive Plus* to *Q-Exactive Plus*

- Installation pending
Q-Exactive plus

MRM  DDMS

DIA

AIF

Q 1  HCD
Metabolomics: Detect the Unexpected!

1. Target analysis
   few metabolites

2. Metabolite profiling
   some selected metabolites

3. Metabolomics
   all metabolites

Metabolic fingerprinting
classifying samples
Environmental Chemicals Screening Strategy

Targeted (Known compounds)

1. Chemical structures known
2. Standards and Retention times available

Xcalibur Qual Browser layout search and PBC library search

Targeted are confirmed

Non-targeted (Targeted unknowns)

1. Chemical structures known
2. Standards and RTs may be available

Try Xcalibur layout search DBC, TCF library search

Putative hit-list generated

Non-targeted Unknown (Unknown unknowns)

1. Chemical structures may be known
2. Standards and RTs may be available

DBC, TCF library search
Statistical analysis ChemSpider search

Putative hit-list generated
Expanding BEST Analysis Update

**Blood Samples:** n=315

- Metals: 250

**Urine Samples:** n=218

- OP specific metabolites, pyrethroids & herbicides: 218
- Creatinine: 83
- Environmental phenols: 20
- Phthalate metabolites: 198
- Metals: 83
- OH-PAHs: 20
- Perchlorate: 218
- *Arsenic Speciation (TBD): 57

*Analyses Pending*

*Total # of samples analyzed*  
*Total # of samples awaiting analysis*

*Samples are only analyzed if total urinary arsenic levels are ≥20µg/L*
CDC Biomonitoring Proficiency Testing

<table>
<thead>
<tr>
<th>Phthalates</th>
<th>Polycyclic aromatic hydrocarbons (PAHs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>• mono-n-butyl phthalate (mBP)</td>
<td>• 1-hydroxynaphthalene (1-NAP)</td>
</tr>
<tr>
<td>• mono-3-carboxypropyl phthalate (mCPP)</td>
<td>• 2-hydroxynaphthalene (2-NAP)</td>
</tr>
<tr>
<td>• monoethyl phthalate (mEP)</td>
<td>• 2-hydroxyfluorene (2-FLU)</td>
</tr>
<tr>
<td>• mono-2-ethyl-5-carboxypentyl phthalate (mECPP)</td>
<td>• 3-hydroxyfluorene (3-FLU)</td>
</tr>
<tr>
<td>• monobenzyl phthalate (mBzP)</td>
<td>• 9-hydroxyfluorene (9-FLU)</td>
</tr>
<tr>
<td>• mono-2-ethylhexyl phthalate (mEHP)</td>
<td>• 1-hydroxyphenanthrene (1-PHE)</td>
</tr>
<tr>
<td>• mono-2-ethyl-5-hydroxyhexyl phthalate (mEHHP)</td>
<td>• 2-hydroxyphenanthrene (2-PHE)</td>
</tr>
<tr>
<td>• mono-2-ethyl-5-oxohexyl phthalate (mEOHP)</td>
<td>• 3-hydroxyphenanthrene (3-PHE)</td>
</tr>
<tr>
<td>• mono-isobutyl phthalate (miBP)</td>
<td>• 1-hydroxypyrene (1-PYR)</td>
</tr>
</tbody>
</table>

### CDC Biomonitoring Proficiency Testing (2)

<table>
<thead>
<tr>
<th>Environmental Phenols</th>
<th>Universal Pesticides</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bisphenol A (BPA)</td>
<td>3,5,6-trichloro-2-pyridinol (TCPy)</td>
</tr>
<tr>
<td>2,4-dichlorophenol</td>
<td>3-phenoxybenzoic acid (3-PBA)</td>
</tr>
<tr>
<td>2,5-dichlorophenol</td>
<td>2-Isopropyl-4-methyl-6-hydroxypyrimidine (IMPY)</td>
</tr>
<tr>
<td>benzophenone-3 (BP-3)</td>
<td>Trans-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropane-1-carboxylic acid (trans-DCCA)</td>
</tr>
<tr>
<td>Triclosan</td>
<td>4-fluoro-3-phenoxy-benzoic acid (4F-3-PBA)</td>
</tr>
<tr>
<td>methyl-paraben</td>
<td>2,4-dichlorophenoxyacetic acid</td>
</tr>
<tr>
<td>ethyl-paraben</td>
<td>2,4,5-trichlorophenoxyacetic acid</td>
</tr>
<tr>
<td>propyl-paraben</td>
<td></td>
</tr>
<tr>
<td>butyl paraben</td>
<td></td>
</tr>
</tbody>
</table>

EHL success rate for last CDC PT event = 97%
• Exposures to environmental phenols in California firefighters and findings of elevated urinary benzophenone-3 levels (submitted to *Environ. Health Perspect.*)

• Validation of a simple and robust method for arsenic speciation in human urine using HPLC-ICP-MS (submitted to *Journal of AOAC International*)

• Method development for the simultaneous analysis of *trans, trans*-muconic acid, 1, 2-dihydroxybenzene, *S*-phenylmercapturic acid and *S*-benzylmercapturic acid in human urine by liquid chromatography/tandem mass spectrometry (in press, *Analytical Method*)

❖ Visit the [Biomonitoring CA website](#) for a list of all publications
Future work

- Methods development and validation
- Collaboration with Kaiser Permanente Northern California (KPNC) Division of Research
- Analyses of GDSP maternal serum samples