



Using the US EPA's CompTox Chemistry Dashboard to support identification and screening of emerging contaminants in the environment

*Andrew D. McEachran**, Seth Newton, Mark Strynar, Rebecca McMahan, Melanie Hedgespeth, Damian Shea, Jon R. Sobus, Elizabeth G. Nichols, Antony J. Williams

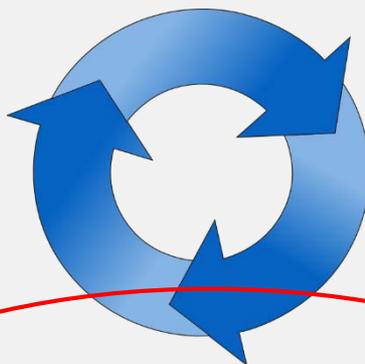
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The General Approach

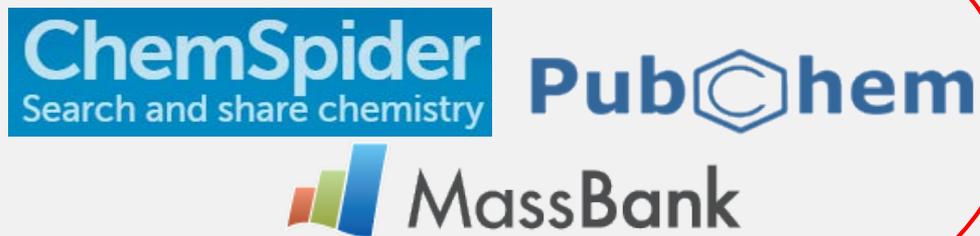
Analytical Instruments



Comp. Tools & Workflows

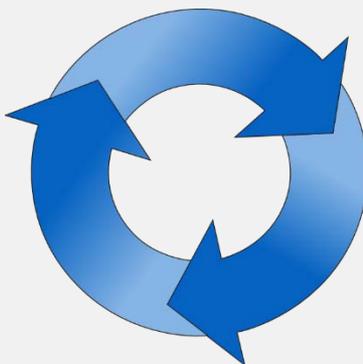


Databases



The General Approach

Analytical Instruments



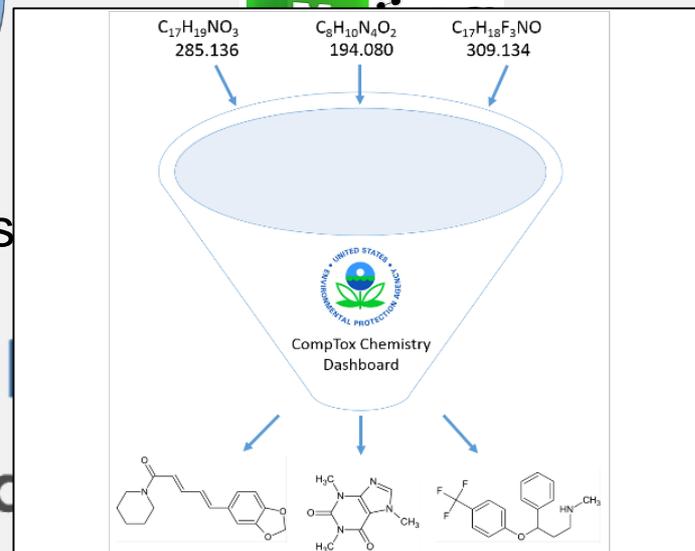
Databases

ChemSpider
Search and share chemistry

Pub

MassBo

Comp. Tools & Workflows



CompTox Chemistry Dashboard

<https://comptox.epa.gov>



Chemistry Dashboard

Search a chemical by systematic name, synonym, CAS number, or InChIKey



Single component search Ignore isotopes

See what people are saying, read the dashboard comments!

Need more? Use advanced search.



Searching for unknowns in the Dashboard

Chemistry Dashboard

Advanced Search

Mass Search

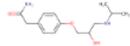
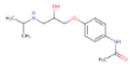
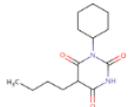
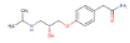
266.163  amu ±

Single component Ignore isotopes

Search Results

 Searched by Mass and single component chemicals: Found 47 results for '266.163 ± 5 ppm'.

Download as:

ID ↑↓	Structure	Preferred Name ↑↓	CAS-RN ↑↓	QC Level ↑↓	CPCat Count	Number of S...	PubChem D...	Monoisotopic Mass ↑↓	Mass Differenc...
DTXSID2022628 ToxCast™		Atenolol	29122-68-7	Level 2: Expert curat...	4	46	185	266.163043	0.0000 <input type="checkbox"/>
DTXSID0021179 ToxCast™		Practolol	6673-35-4	Level 2: Expert curat...	0	32	92	266.163043	0.0000 <input type="checkbox"/>
DTXSID4048854 ToxCast™		Bucolome	841-73-6	Level 2: Expert curat...	0	20	28	266.163043	0.0000 <input type="checkbox"/>
DTXSID0045753 ToxCast™		R-(+)-Atenolol	56715-13-0	Level 2: Expert curat...	0	19	72	266.163043	0.0000 <input type="checkbox"/>

Molecular Formula Search

Molecular Formula

C14H22N2O3

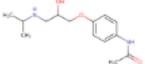
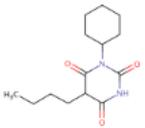
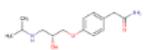
Search 

Single component

Search Results

 Searched by Molecular Formula and single component chemicals: Found 48 results for 'C14H22N2O3'.

Download as: TSV ▾ Excel ▾ SDF ▾

ID ↑↓	Structure	Preferred Name ↑↓	CAS-RN ↑↓	QC Level ↑↓	CPCat Count	Number of S...	PubChem D...	Monoisotopic Mass
DTXSID2022628 ToxCast™ 		Atenolol	29122-68-7	Level 2: Expert curat...	4	46	185	266.163043 
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Identifying known unknowns using the US EPA's CompTox Chemistry Dashboard

Andrew D. McEachran¹ · Jon R. Sobus² · Antony J. Williams³

- On same 162 chemicals, Dashboard outperforms ChemSpider

	Mass-based searching		Formula-based searching	
	Dashboard	ChemSpider	Dashboard	ChemSpider
Average rank position	1.3	2.2 ^a	1.2	1.4
Percent in #1 position	85%	70%	88%	80%

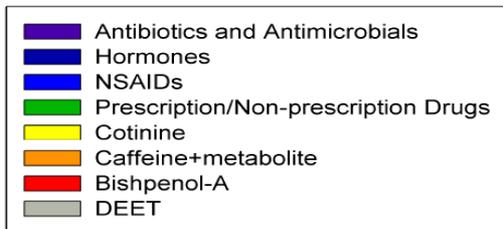
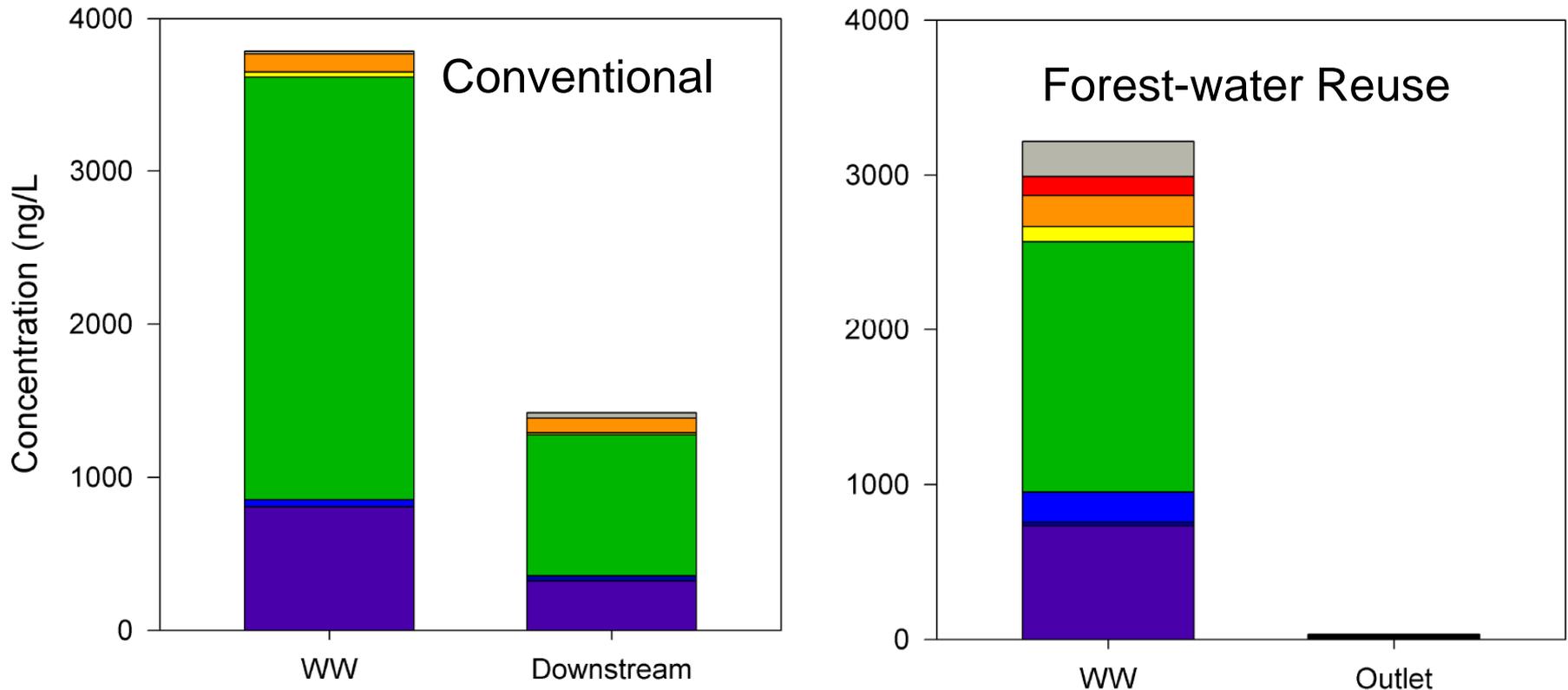
^a Average rank in ChemSpider shown here does not include an outlier where the rank was 201, when added the average rank position is 3.5

Application to environmental samples

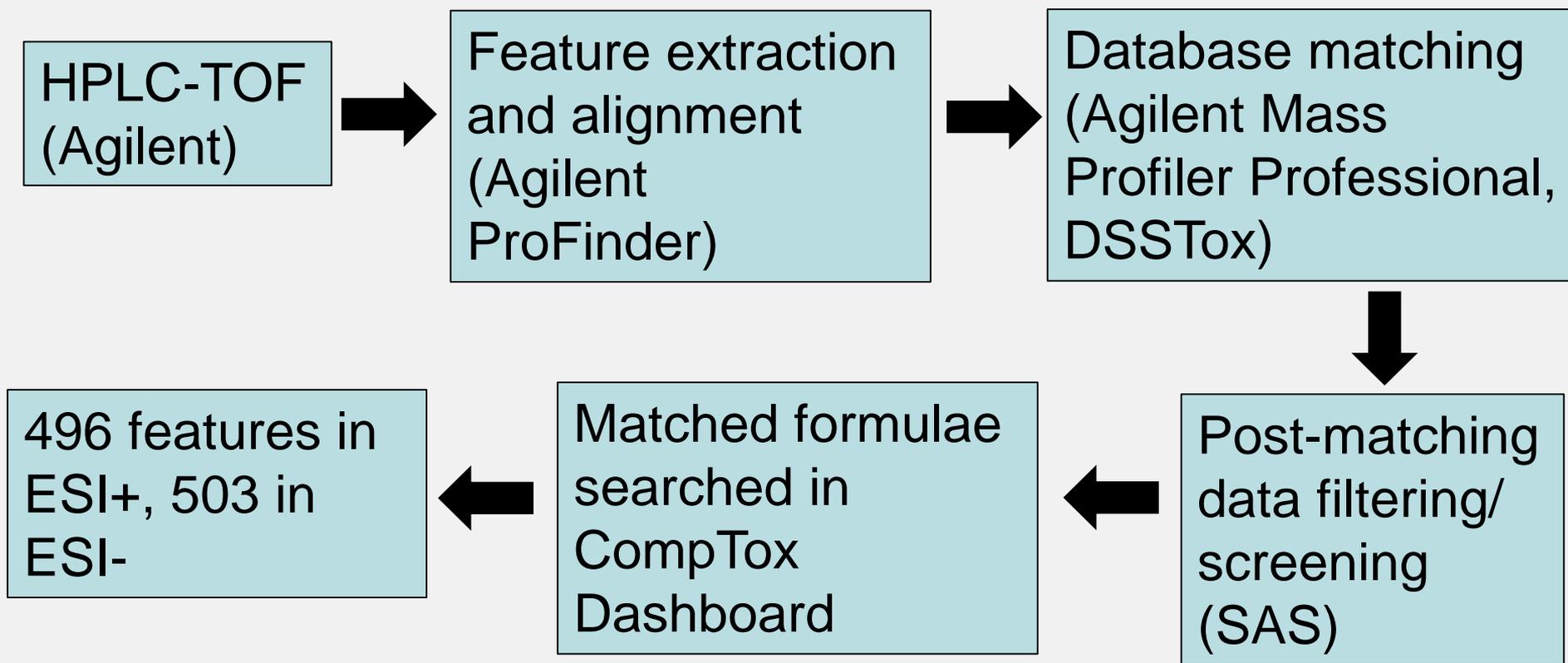
Forested wastewater land application



Total summed PPCP concentrations greater downstream of conventional system



Non-targeted analysis workflow



Average DB-Matched Chemicals per site/location

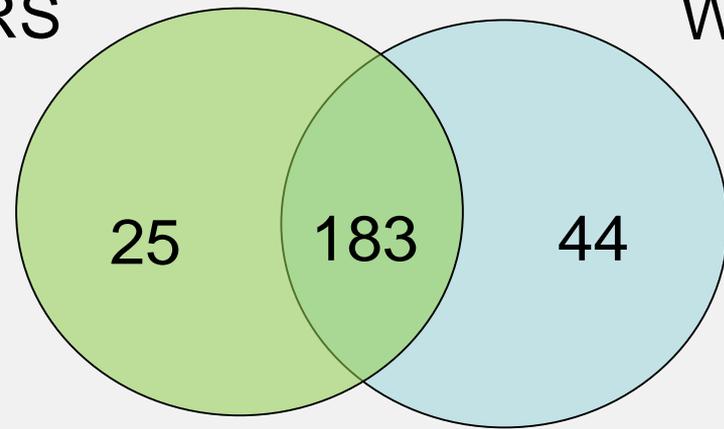
	FWRS	WWTP
Upstream	128	132
Wastewater	367	460
Downstream	123	202

FWRS= Forest-water Reuse System
WWTP=Wastewater Treatment Plant

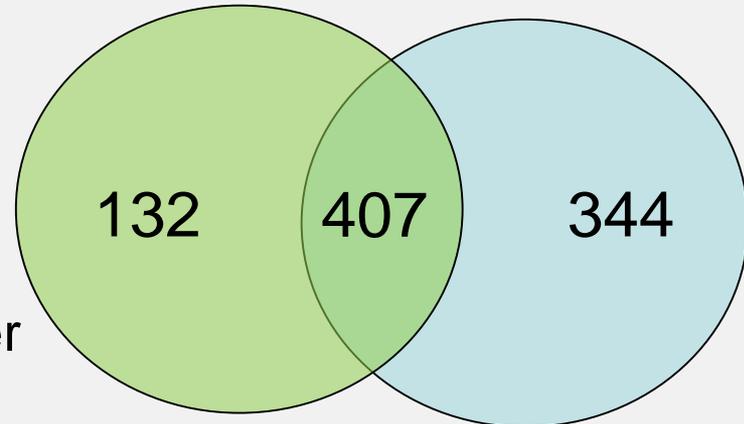
FWRS

WWTP

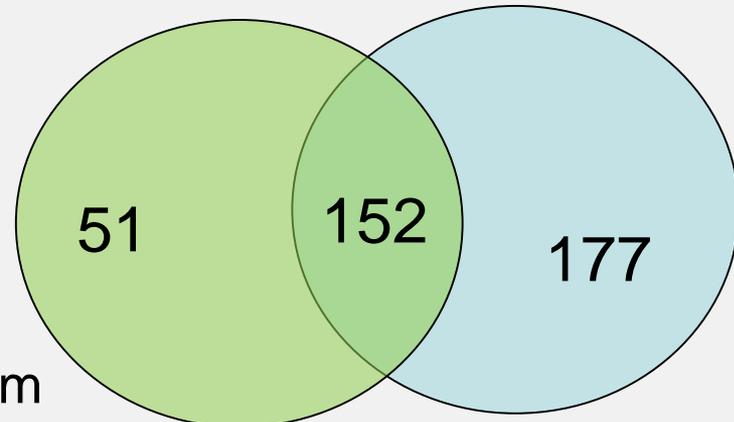
Upstream



Wastewater

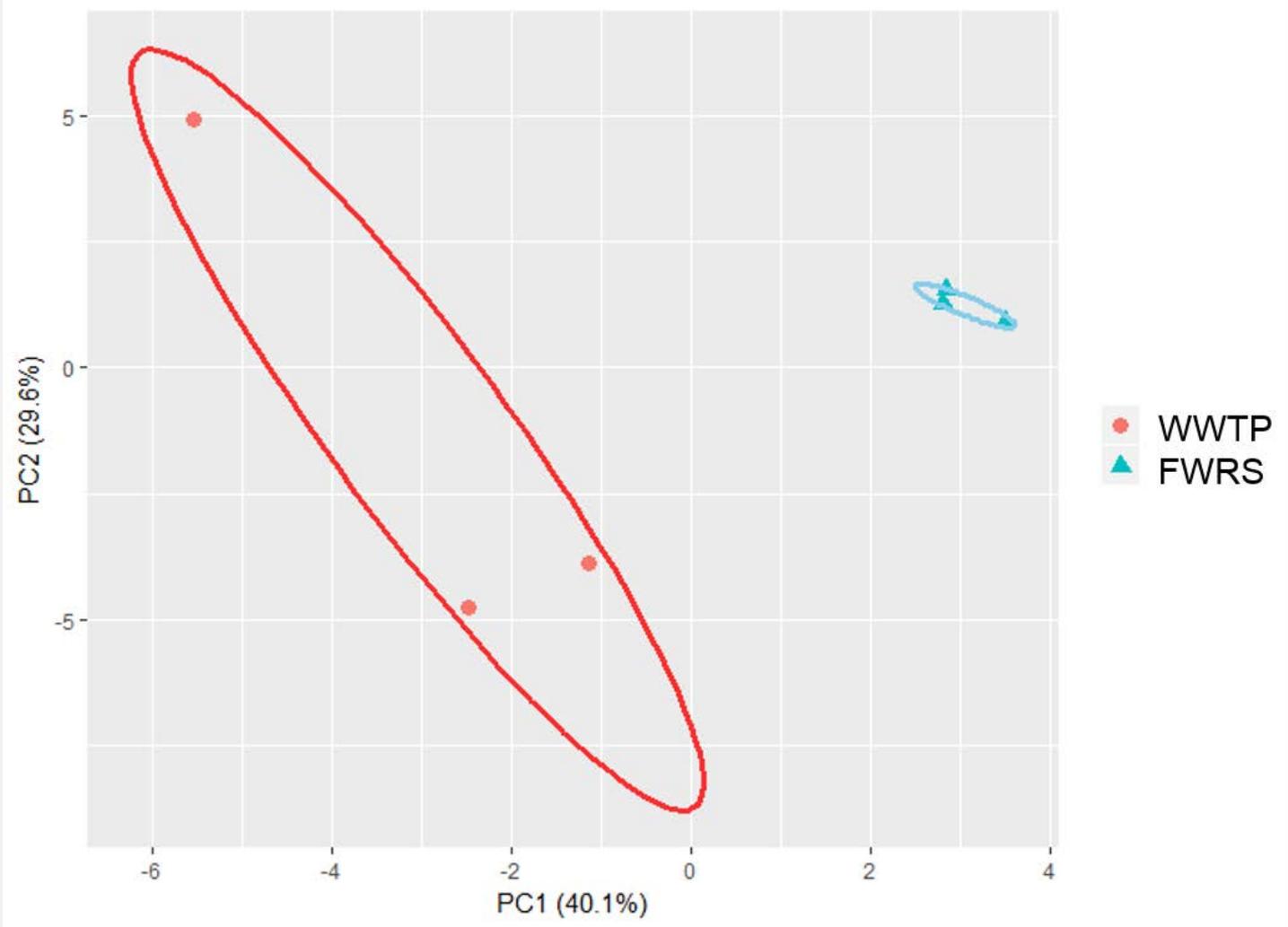


Downstream



Number of
unique/similar
matched
chemicals
between sites

Overall chemical composition in wastewater is distinct between treatment sites





Tentative
Candidates:
Top 50 most
frequently
occurring in
ESI-



Tentative
Candidates:
Top 50 most
frequently
occurring in
ESI+



Conclusions

- Structure identification in NTA requires integration of many resources
- The US EPA's CompTox Chemistry Dashboard provides data and functionality for environmental chemists using HRMS and NTA
- Using the Dashboard, analysis of wastewaters and water-reuse systems is ongoing

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Jeff Edwards

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Jennifer Smith

EPA NERL

Katherine Phillips

Kristin Isaacs

Kathie Dionisio

Jon Sobus

Mark Strynar

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Sarah Laughlin-Toth*

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