



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*

ENVR 136

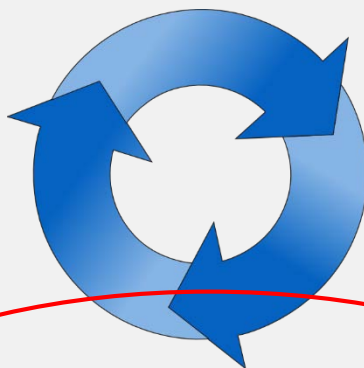
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The General Approach

Analytical Instruments



Comp. Tools & Workflows

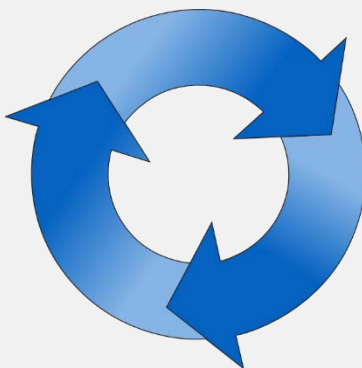


Databases



The General Approach

Analytical Instruments



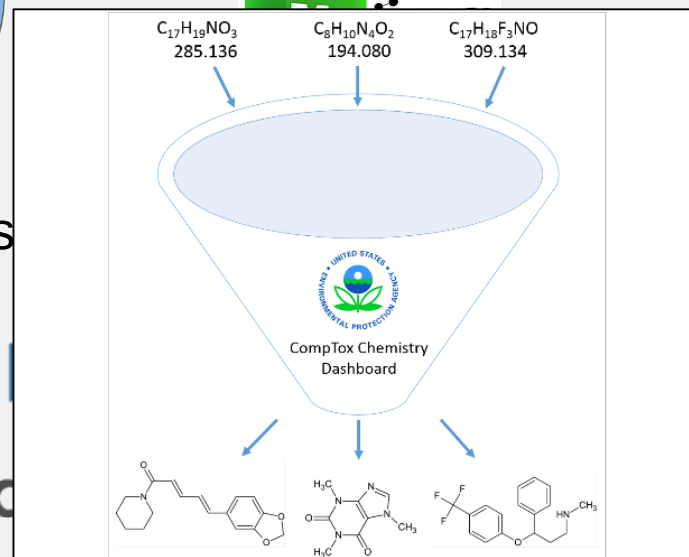
Databases

ChemSpider
Search and share chemistry

Pul

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.

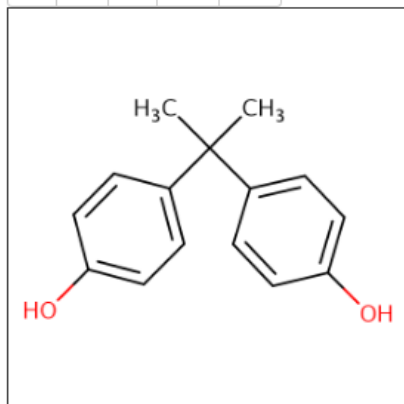


CompTox Chemistry Dashboard

Bisphenol A

80-05-7 | DTXSID7020182

© Searched by Expert Validated Synonym: Found 1 result for 'bpa'.



Wikipedia

Bisphenol A (BPA) is an organic synthetic compound with the chemical formula $(\text{CH}_3)_2\text{C}(\text{C}_6\text{H}_4\text{OH})_2$ belonging to the group of diphenylmethane derivatives and bisphenols, with two hydroxyphenyl groups. It is a colorless solid that is soluble in organic solvents, but poorly soluble in water. It has been in commercial use since 1957. BPA is employed to make certain plastics and epoxy resins. BPA-based plastic is clear and tough... [Read more](#)

Intrinsic Properties

Structural Identifiers

Related Compounds (Beta)

Presence in Lists

Record Information

CompTox Chemistry Dashboard

Bisphenol A

80-05-7 | DTXSID7020182

© Searched by Expert Validated Synonym: Found 1 result for 'bpa'.

Chemical Properties

Env. Fate/Transport

Synonyms

External Links

Toxicity Values (Beta)

Exposure

Bioassays

Similar Molecules (Beta)

Literature

Comments

Summary

LogP: Octanol-Water

Water Solubility

Density

Melting Point

Boiling Point

Surface Tension

Vapor Pressure

LogKoa: Octanol-Air

Henry's Law

Index of Refraction

Download as:

TSV

Excel

SDF

Property	Average		Median		Range		Unit
	Experimental	Predicted	Experimental	Predicted	Experimental	Predicted	
LogP: Octanol-Water	3.32 (1)	3.24 (4)	3.32 to 3.32	3.24	3.32	2.40 to 3.73	-
Water Solubility	5.26e-04 (1)	1.58e-03 (4)	5.26e-04 to 5.26e-04	1.58e-03	5.26e-04	5.70e-04 to 3.68e-03	mol/L
Density	-	1.14 (1)	-	1.14	-	-	g/cm ³
Melting Point	155 (7)	144 (3)	153 to 158	144	153 to 158	132 to 157	°C
Boiling Point	200 (1)	349 (3)	200 to 200	349	200	334 to 364	°C
Surface Tension	-	46.0 (1)	-	46.0	-	-	dyn/cm
Vapor Pressure	-	2.52e-07 (3)	-	2.52e-07	-	7.01e-08 to 5.34e-07	mmHg
LogKoa: Octanol-Air	-	8.38 (1)	-	8.38	-	-	-
Henry's Law	-	6.96e-07 (1)	-	6.96e-07	-	-	atm-m ³ /mole
Index of Refraction	-	1.60 (1)	-	1.60	-	-	-
Molar Refractivity	-	68.2 (1)	-	68.2	-	-	cm ³
pKa Acidic Apparent	-	10.3 (1)	-	10.3	-	-	-
Molar Volume	-	200 (1)	-	200	-	-	cm ³

CompTox Chemistry Dashboard

Bisphenol A

80-05-7 | DTXSID7020182

Chemical Properties

Env. Fate/Transport

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Toxicity Values (Beta)

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Bioassays

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Literature

Comments

Chemical Weight Fracti..

Product Use Categories...

Chemical Functional Us...

Monitoring Data

Exposure Predictions

Download as:

TSV

Excel

279th highest exposure ⓘ

ⓘ Exposure Predictions (mg/kg-bw/day)

	Ages 6-11	Ages 12-19	Ages 20-65	Ages 65+	BMI > 30	BMI < 30	Repro. Age Females ⓘ	Females	Males	Total
Median	6.30e-05	2.68e-05	2.05e-05	1.61e-05	1.69e-05	2.67e-05	1.11e-05	1.11e-05	3.89e-05	2.11e-05
95th Percentile	5.82e-03	2.00e-03	1.61e-03	2.18e-03	1.45e-03	2.26e-03	1.57e-03	9.09e-04	3.34e-03	2.00e-03

CompTox Chemistry Dashboard

Predicted Probability of Associated Functional Use 

QSAR Version/Date: 2015-11-06

Download as:

[Harmonized Functional Use](#)

[Probability](#)

skin_protectant	0.66
hair_conditioner	0.58
antimicrobial	0.57
masking_agent	0.55
skin_conditioner	0.53
antioxidant	0.51
colorant	0.50
uv_absorber	0.44
soluble_dye	0.43
hair_dye	0.42
crosslinker	0.42
photoinitiator	0.41
humectant	0.41
additive_for_rubber	0.41

Chemical Weight Fraction (Beta)

Product Use Categories (Beta)

Chemical Functional Use (Beta)

Monitoring Data

Exposure Predictions

CompTox Chemistry Dashboard

Chemical Properties	Env. Fate/Transport	Synonyms	External Links	Toxicity Values (Beta)	Exposure	Bioassays	Similar Molecules (Beta)	Literature	Comments
General  EPA Substance Registry Service  NIST Chemistry Webbook  Household Products Database  PubChem  ChempSpider  HMDB  Wikipedia  MSDS Lookup  ToxPlanet  ChemHat: Hazards and Alternat...  ChEMBL  Consumer Product Information ...  ECHA Brief Profile  ECHA Infocard  Sigma-Aldrich Chemicals  Wikidata  Wolfram Alpha  WebWISER  ECHA Dossier	Toxicology  ACToR  DrugPortal  CCRIS  ChemView  CTD  eChemPortal  EDSP Dashboard  Gene-Tox  HSDB  ToxCast Dashboard 2  LactMed  International Toxicity Estimates ...  ACToR PDF Report	Publications  Toxline  Environmental Health Perspecti...  NIEHS  National Toxicology Program  Google Books  Google Scholar  Google Patents  PubMed  BioCaddie DataMed  Federal Register  Regulations.gov  RSC Publications  Springer Materials  IRIS Assessments  CORE Literature Search  Bielefeld Academic Search Engi...	Analytical  RSC Analytical Abstracts  FOR-IDENT  MONA: MassBank North America  NEMI: National Environmental M...  Tox21 Analytical Data	Prediction  Chemicalize  Proton NMR Prediction  Carbon-13 NMR Prediction  2D NMR HSQC/HMBC Prediction  ChemRTP Predictor					

Searching for unknowns in the Dashboard

Chemistry Dashboard

Advanced Search

Mass Search

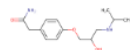
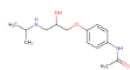
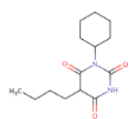
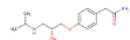
266.163  amu ±

☒ 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	
DTXSID0021179	ToxCast™  	Practolol	6673-35-4	Level 2: Expert curat...	0	32	92	266.163043	0.0000	
DTXSID4048854	ToxCast™  	Bucolome	841-73-6	Level 2: Expert curat...	0	20	28	266.163043	0.0000	
DTXSID0045753	ToxCast™  	R-(+)-Atenolol	56715-13-0	Level 2: Expert curat...	0	19	72	266.163043	0.0000	

Molecular Formula Search

Molecular Formula

C14H22N2O3

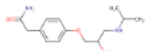
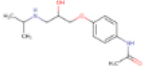
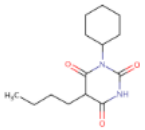
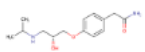
Search 

☒ 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 
DTXSID0021179 ToxCast™ 		Practolol	6673-35-4	Level 2: Expert curat...	0	32	92	266.163043 
DTXSID4048854 ToxCast™ 		Bucolome	841-73-6	Level 2: Expert curat...	0	20	28	266.163043 
DTXSID0045753 ToxCast™ 		R-(+)-Atenolol	56715-13-0	Level 2: Expert curat...	0	19	72	266.163043 

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

MS-Ready structures

- De-salted, de-solvated, no stereochemistry, separation of mixtures and multi-component structures

	A	B	C	D	E	F
1	INPUT	DTXSID	CASRN	PREFERRED NAME	MOL FORMULA	MONOISOTOPIC MASS
2	C6H6O	DTXSID5021124	108-95-2	Phenol	C6H6O	94.041864813
3	C6H6O	DTXSID4027072	139-02-6	Sodium phenolate	C6H5NaO	116.02380906
4	C6H6O	DTXSID8073261	1487-18-9	Furan, 2-ethenyl-	C6H6O	94.041864813
5	C6H6O	DTXSID10219242	6921-27-3	2-Propynyl ether	C6H6O	94.041864813
6	C6H6O	DTXSID10183353	291-70-3	Oxepin	C6H6O	94.041864813
7	C6H6O	DTXSID7064073	5973-17-1	Phenol, ammonium salt	C6H9NO	111.068413914
8	C6H6O	DTXSID90363757	6569-83-1	7-oxabicyclo[2.2.1]hepta-2,5-diene	C6H6O	94.041864813
9	C6H6O	DTXSID60179347	24599-57-3	2,4-Cyclohexadienone	C6H6O	94.041864813
10	C6H6O	DTXSID5070109	64601-04-3	Phenol, compd. with 2-aminoethanol (1:1)	C8H13NO2	155.094628663
11	C6H6O	DTXSID9075294	2122-46-5	Phenoxy	C6H5O	93.034039781
12						

Batch Searching of Unknowns

Batch Search

Please enter one identifier per line

Select Input Type(s)

- ☐ Chemical Name
- ☐ CAS-RN
- ☐ InChIKey
- ☐ DSSTox Substance ID
- ☒ Exact Molecular Formula 

Include top

hits in download

Enter Identifiers to Search

C14H22N2O3
C18H34N2O6S
C10H12N2O
C14H18N4O3
C12H11N7
C8H9NO2
C7H8N4O2
C38H72N2O12
C17H21NO
C8H10N4O2

Display All Chemicals

Download Chemical Data

Select Output Format

Excel ▼

Customize Results

☐ Select All

Chemical Identifiers

- ☒ Chemical Name
- ☒ DTXSID
- ☒ CAS-RN
- ☐ InChIKey
- ☐ IUPAC Name

Metadata

- ☐ Curation Level Details
- ☒ Data Sources
- ☐ Assay Hit Count
- ☐ NHANES/Predicted Exposure
- ☐ Include ToxVal Data Availability

Structures

- ☐ Mol File
- ☐ SMILES
- ☐ InChI String

Intrinsic And Predicted Properties

- ☒ Molecular Formula
- ☐ Average Mass
- ☒ Monoisotopic Mass
- ☐ OPERA and TEST Model Predictions

Download 

Batch Searching of Unknowns

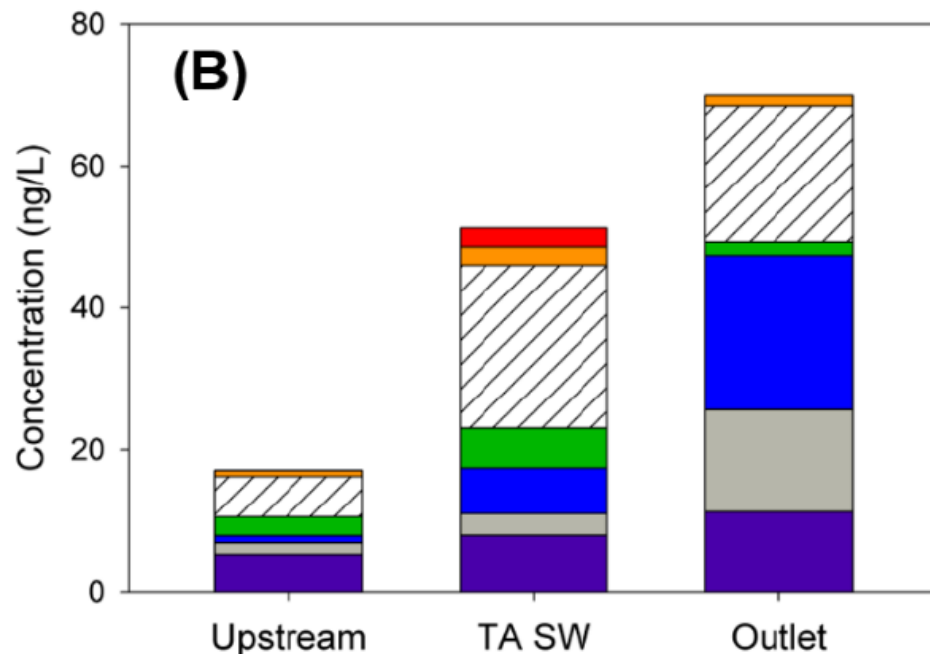
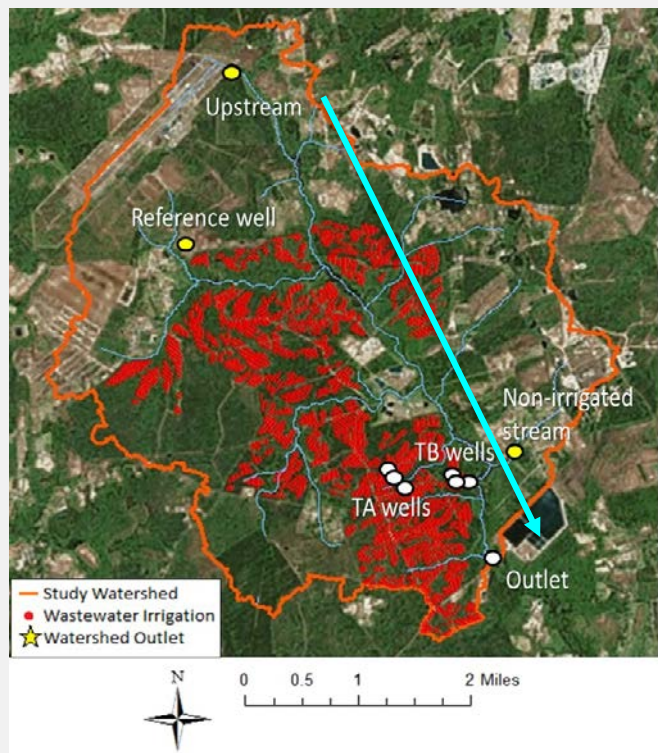
	A	B	C	D	E	F	G
1	INPUT	DTXSID	CASRN	PREFERRED NAME	MOL FORMULA	MONOISOTOPIC MASS	DATA SOURCES
2	C14H22N2O3	DTXSID2022628	29122-68-7	Atenolol	C14H22N2O3	266.163042576	46
3	C14H22N2O3	DTXSID0021179	6673-35-4	Practolol	C14H22N2O3	266.163042576	32
4	C14H22N2O3	DTXSID4048854	841-73-6	Bucolome	C14H22N2O3	266.163042576	20
5	C14H22N2O3	DTXSID1045407	13171-25-0	Trimetazidine dihydrochloride	C14H24Cl2N2O3	338.116398	19
6	C14H22N2O3	DTXSID0045753	56715-13-0	R-(+)-Atenolol	C14H22N2O3	266.163042576	19
7	C14H22N2O3	DTXSID2048531	5011-34-7	Trimetazidine	C14H22N2O3	266.163042576	14
8	C14H22N2O3	DTXSID10239405	93379-54-5	Esatenolol	C14H22N2O3	266.163042576	12
9	C14H22N2O3	DTXSID50200634	52662-27-8	N-(2-Diethylaminoethyl)-2-(4-hydroxyphenoxy)acetamide	C14H22N2O3	266.163042576	7
10	C14H22N2O3	DTXSID4020111	51706-40-2	dl-Atenolol hydrochloride	C14H23ClN2O3	302.1397203	6
11	C14H22N2O3	DTXSID1068693	51963-82-7	Benzenamine, 2,5-diethoxy-4-(4-morpholinyl)-	C14H22N2O3	266.163042576	5
12	C18H34N2O6S	DTXSID3023215	154-21-2	Lincomycin	C18H34N2O6S	406.213757997	35
13	C18H34N2O6S	DTXSID7047803	859-18-7	Lincomycin hydrochloride	C18H35ClN2O6S	442.1904357	22
14	C18H34N2O6S	DTXSID20849438	1398534-62-7	PUBCHEM_71432748	C18H35ClN2O6S	442.1904357	1
15	C10H12N2O	DTXSID1047576	486-56-6	Cotinine	C10H12N2O	176.094963014	40
16	C10H12N2O	DTXSID8075330	50-67-9	Serotonin	C10H12N2O	176.094963014	22
17	C10H12N2O	DTXSID8044412	2654-57-1	4-Methyl-1-phenylpyrazolidin-3-one	C10H12N2O	176.094963014	18
18	C10H12N2O	DTXSID80165186	153-98-0	Serotonin hydrochloride	C10H13ClN2O	212.0716407	11
19	C10H12N2O	DTXSID2048870	29493-77-4	(4R,5S)-4-methyl-5-phenyl-4,5-dihydro-1,3-oxazol-2-amine	C10H12N2O	176.094963014	10
20	C10H12N2O	DTXSID10196105	443-31-2	6-Hydroxytryptamine	C10H12N2O	176.094963014	9
21	C10H12N2O	DTXSID90185693	31822-84-1	1,4,5,6-Tetrahydro-5-phenoxy pyrimidine	C10H12N2O	176.094963014	7
22	C10H12N2O	DTXSID40178777	2403-66-9	2-Benzimidazolepropanol	C10H12N2O	176.094963014	7
23	C10H12N2O	DTXSID80157026	13140-86-8	N-Cyclopropyl-N'-phenylurea	C10H12N2O	176.094963014	6
24	C10H12N2O	DTXSID30205607	570-14-9	4-Hydroxytryptamine	C10H12N2O	176.094963014	6
25	C14H18N4O3	DTXSID5023900	17804-35-2	Benomyl	C14H18N4O3	290.137890456	68
26	C14H18N4O3	DTXSID3023712	738-70-5	Trimethoprim	C14H18N4O3	290.137890456	51
27	C14H18N4O3	DTXSID40209671	60834-30-2	Trimethoprim hydrochloride	C14H19ClN4O3	326.1145682	8
28	C14H18N4O3	DTXSID70204210	55687-49-5	Benzenemethanol, 4-((2,4-diamino-5-pyrimidinyl)methyl)-2-	C14H18N4O3	290.137890456	5
29	C14H18N4O3	DTXSID20152671	120075-57-2	6-Methoxy-4-(3-(N,N-dimethylamino)propylamino)-5,8-quin	C14H18N4O3	290.137890456	4
30	C14H18N4O3	DTXSID30213742	63931-79-3	1H-1,2,4-Benzotriazepine-3-carboxylic acid, 4,5-dihydro-4-	C14H18N4O3	290.137890456	3
31	C14H18N4O3	DTXSID30219608	69449-07-6	2,4-Pyrimidinediamine, 5-((3,4,5-trimethoxyphenyl)methyl)-	C14H20N4O4	308.14845514	3
32	C14H18N4O3	DTXSID20241155	94232-27-6	L-Aspartic acid, compound with 5-((3,4,5-trimethoxyphenyl)methyl)-	C18H25N5O7	423.175398165	3
33	C14H18N4O3	DTXSID80241156	94232-28-7	L-Glutamic acid, compound with 5-((3,4,5-trimethoxyphenyl)methyl)-	C19H27N5O7	437.191048229	3
34	C14H18N4O3	DTXSID20143781	101204-93-7	1H-Pyrido(2,3-e)-1,4-diazepine-2,3,5-trione, 4-(2-(diethylam	C14H18N4O3	290.137890456	3
35	C12H11N7	DTXSID6021373	396-01-0	Triamterene	C12H11N7	253.107593382	52
36	C12H11N7	DTXSID00204465	5587-93-9	Ampyrimine	C12H11N7	253.107593382	7
37	C12H11N7	DTXSID5064621	7300-26-7	Benzenamine, 4-azido-N-(4-azidophenyl)-	C12H9N7	251.091943318	4
38	C12H11N7	DTXSID00848025	90293-82-6	Sulfuric acid-6-phenylpteridine-2,4,7-triamine (1/1)	C12H13N7O4S	351.074973101	1
39	C12H11N7	DTXSID50575293	92310-83-3	(1E)-N-Phenyl-1,2-bis(1H-1,2,4-triazol-1-yl)ethan-1-imine	C12H11N7	253.107593382	1
40	C8H9NO2	DTXSID2020006	103-90-2	Acetaminophen	C8H9NO2	151.063328534	75
41	C8H9NO2	DTXSID6025567	134-20-3	Methyl 2-aminobenzoate	C8H9NO2	151.063328534	50

Application to environmental samples

Forested wastewater land application



Do Forest Water Reuse Systems Export PPCPs?



	Mean Log Kow
Plasticizer	3.32
Hormones	3.32
Prescription/OTC Drugs	2.61
NSAIDs	2.21
Antibiotics/Antimicrobials	1.94
Cotinine	0.07
Caffeine+metabolite	-0.07

Surface water flow direction

Conventional wastewater treatment

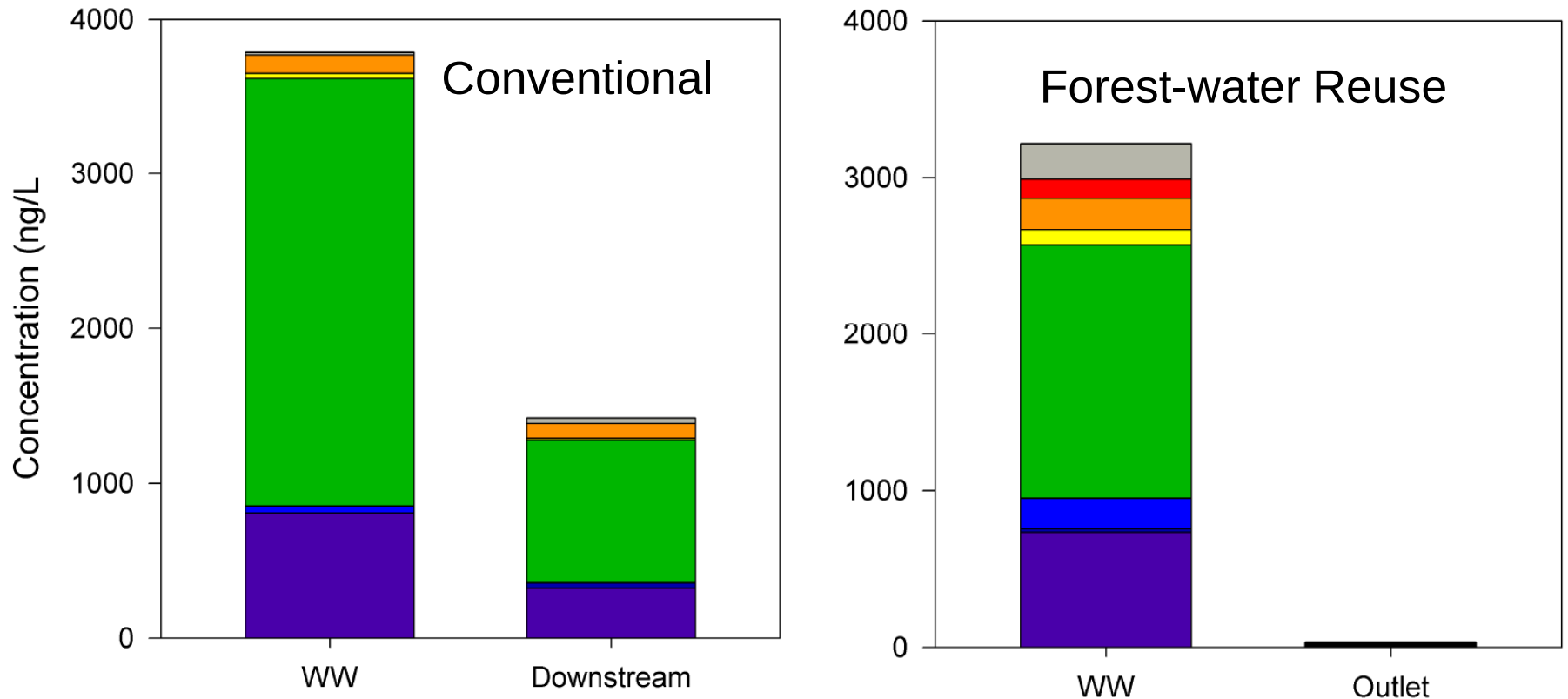
- 6.5 MGD average treatment
- Tertiary treatment with UV disinfection
- Discharge of treated effluent →
- More urbanized area

How does environmental input of emerging contaminants differ between conventional systems and forest-water reuse systems?



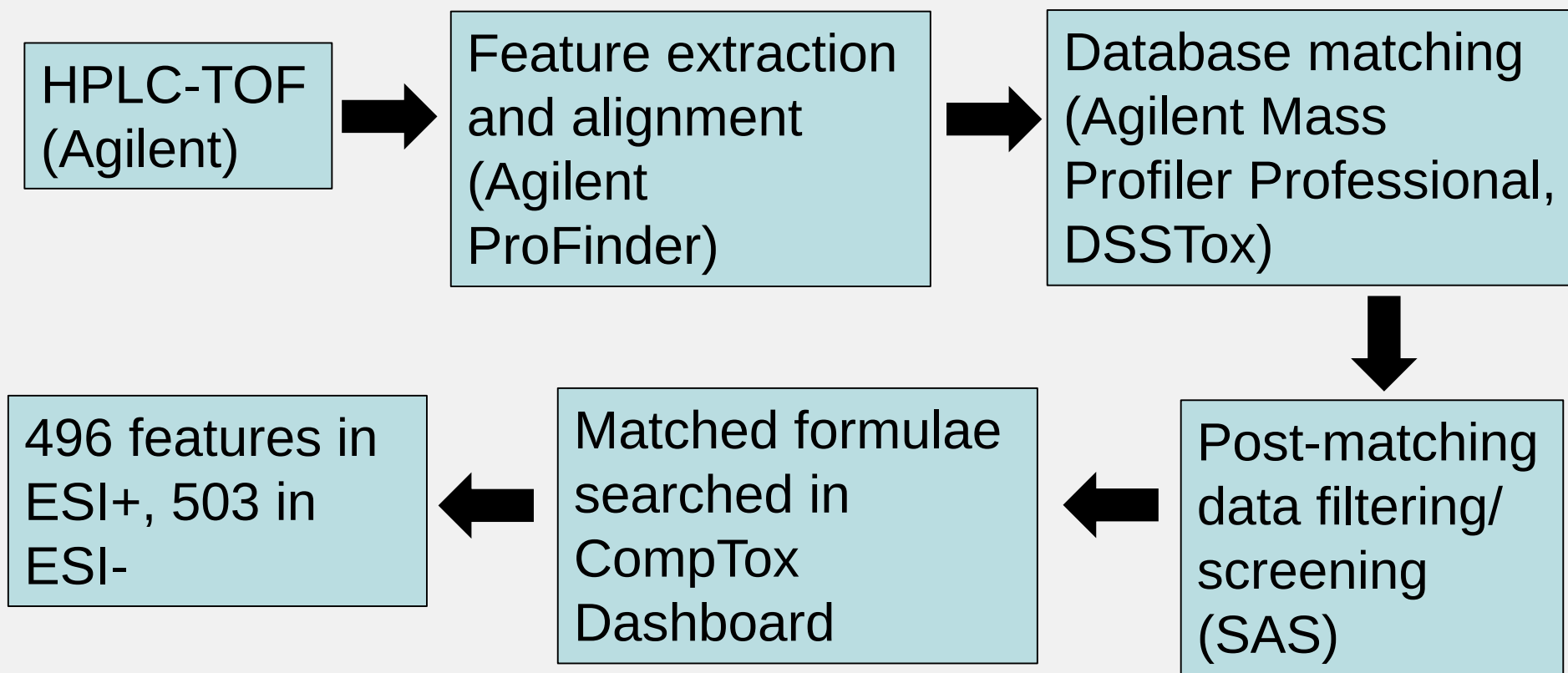
WW release

Total summed PPCP concentrations greater downstream of conventional system



- Antibiotics and Antimicrobials
- Hormones
- NSAIDs
- Prescription/Non-prescription Drugs
- Cotinine
- Caffeine+metabolite
- Bishphenol-A
- DEET

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

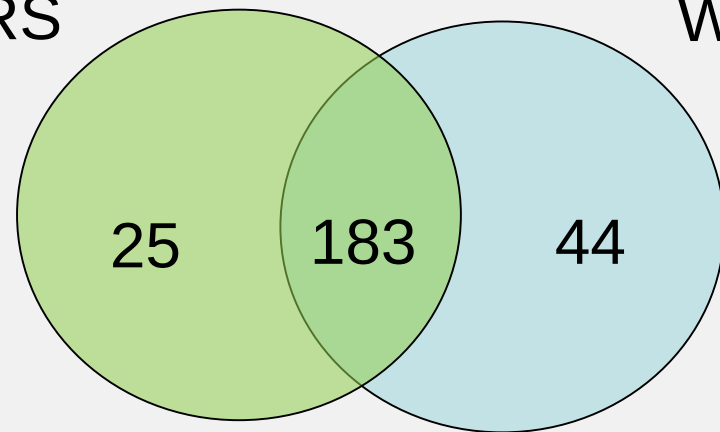
WWTP=Wastewater Treatment Plant

Number of
unique/similar
matched
chemicals
between sites

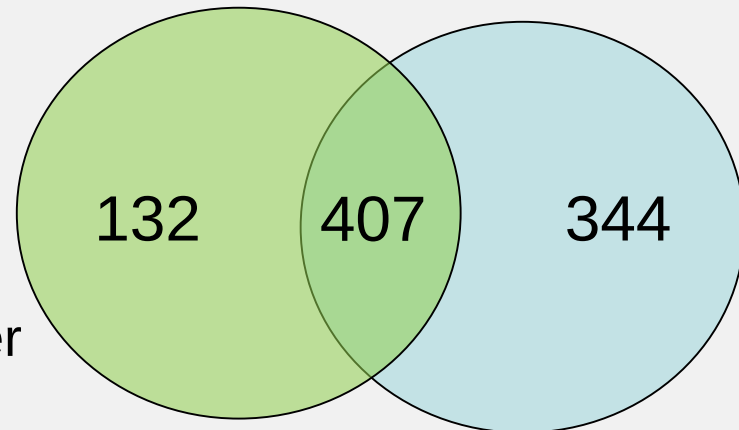
FWRS

WWTP

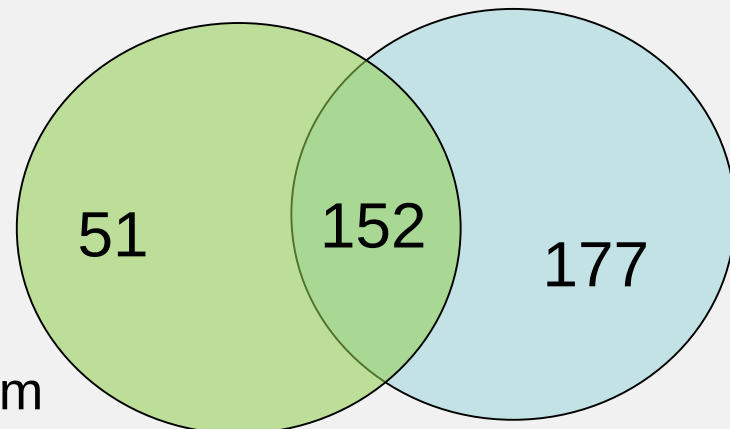
Upstream



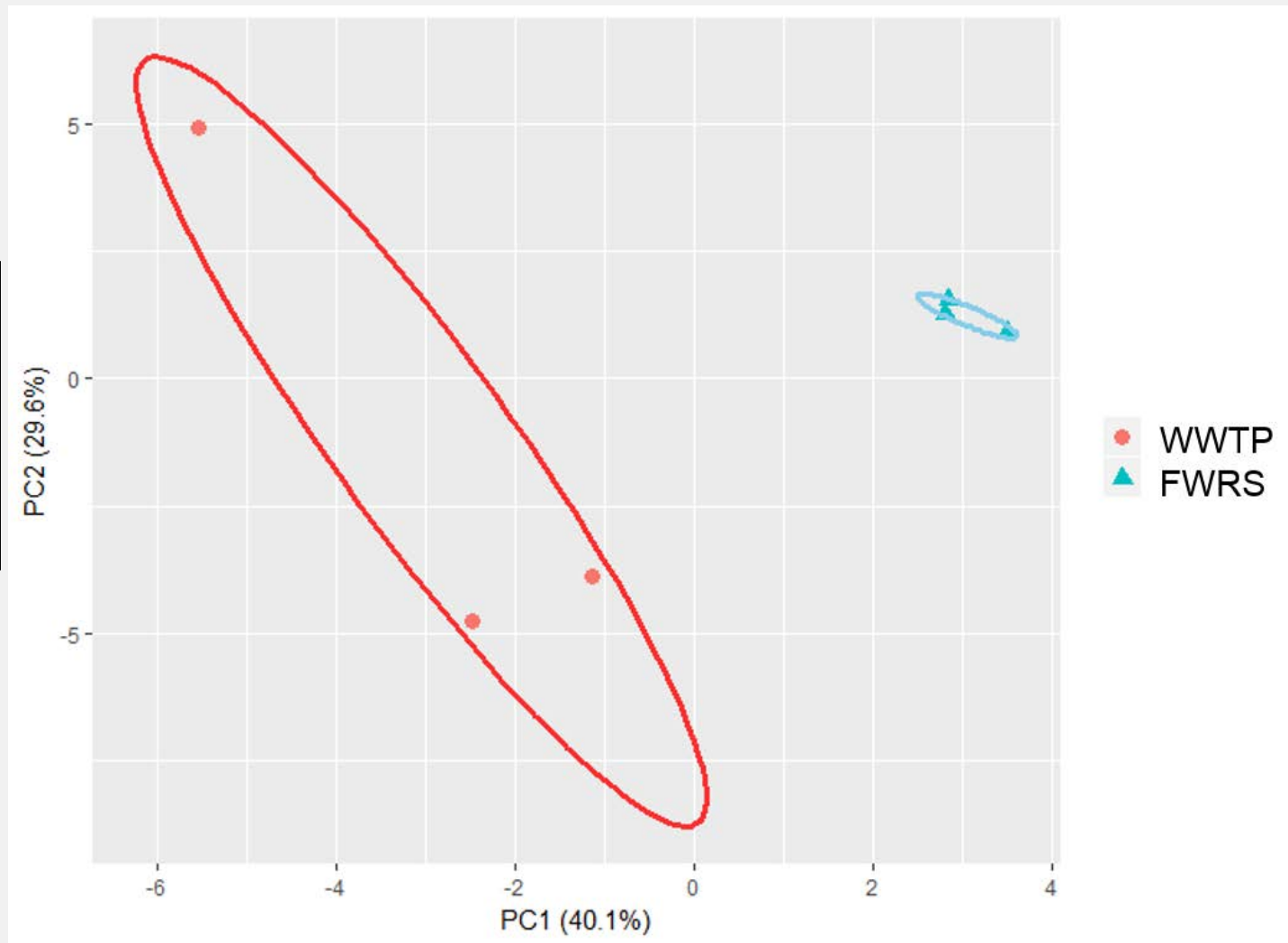
Wastewater



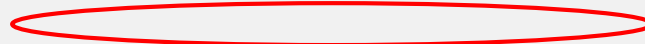
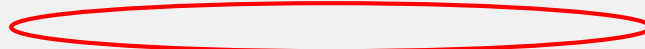
Downstream



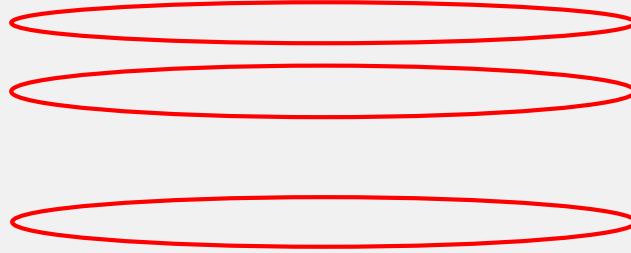
Overall chemical composition in wastewater is distinct between treatment sites



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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- Associated presentations:
 - 4/2 ANYL 76, AJ Williams
 - 4/2 ANYL 77- Poster, AD McEachran
 - 4/6 ENVR 1012, K. Phillips
 - 4/6 ANYL 470, AD McEachran