

Helping Contaminants Emerge: Non-targeted Analysis and Passive Sampling for Assessing Water Quality

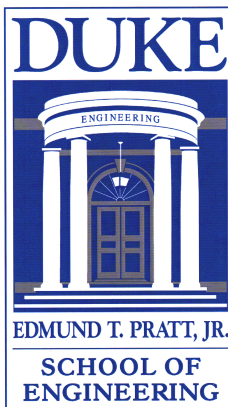
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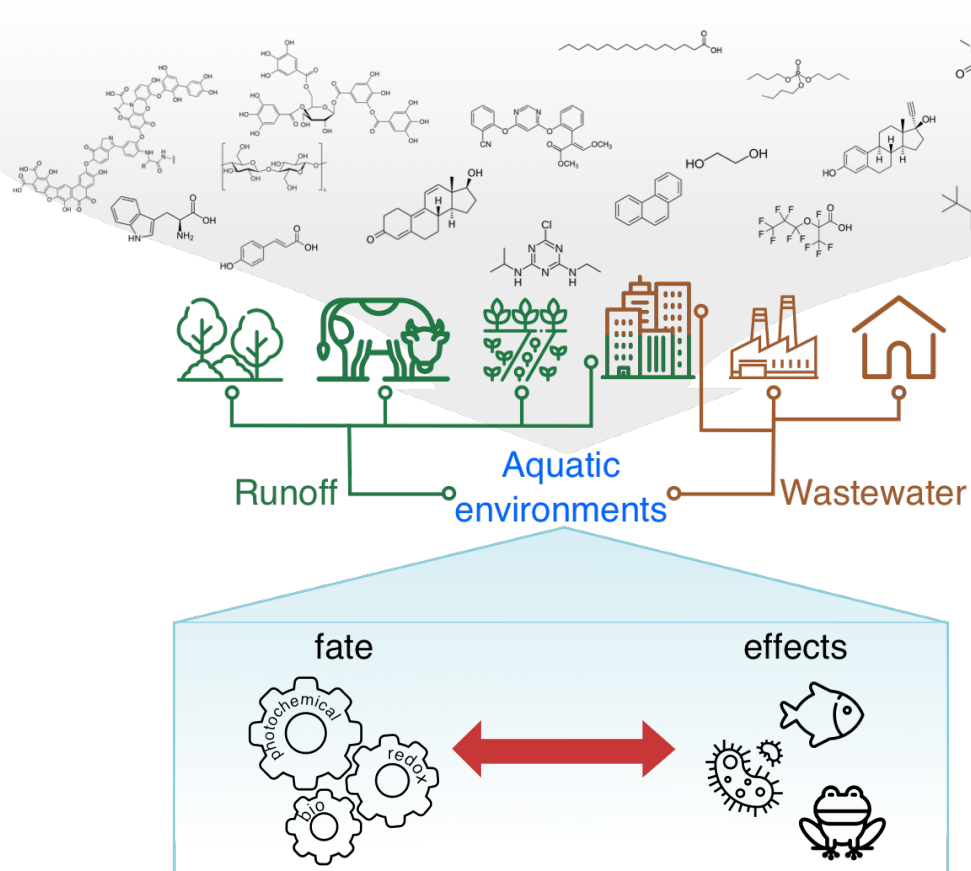
Estuary Institute



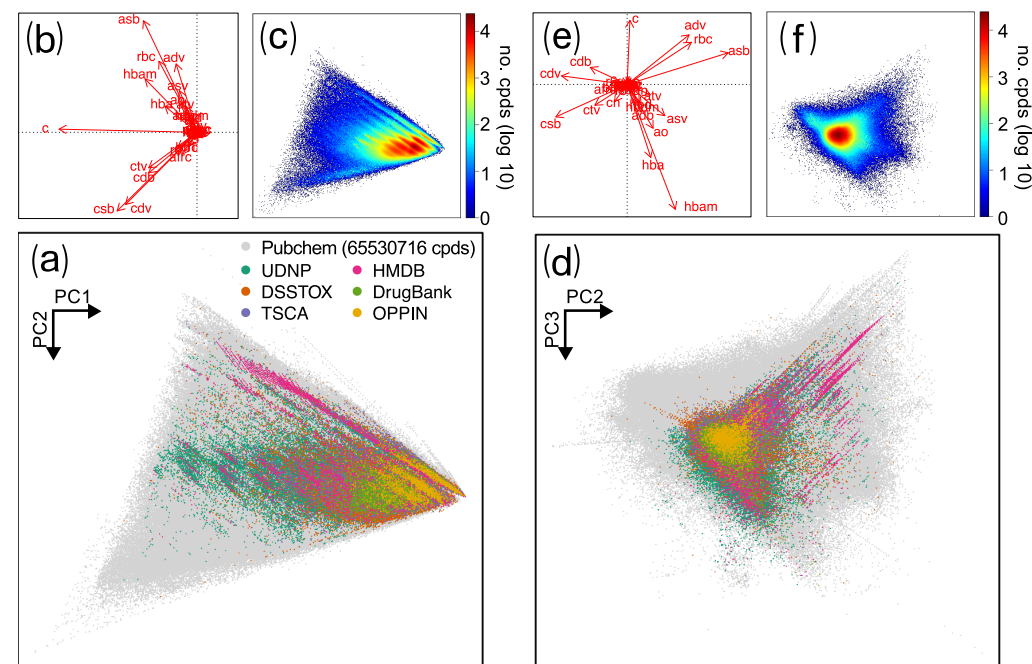
OIMA Brown Bag Webinar, April 26, 2018



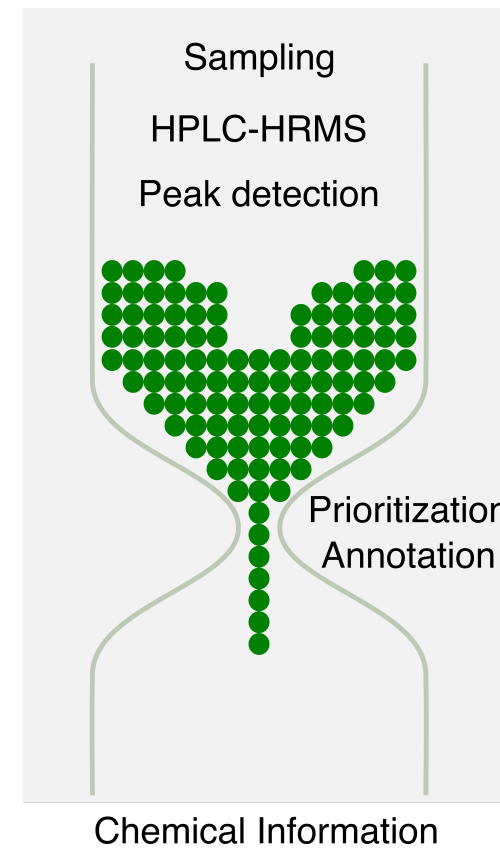
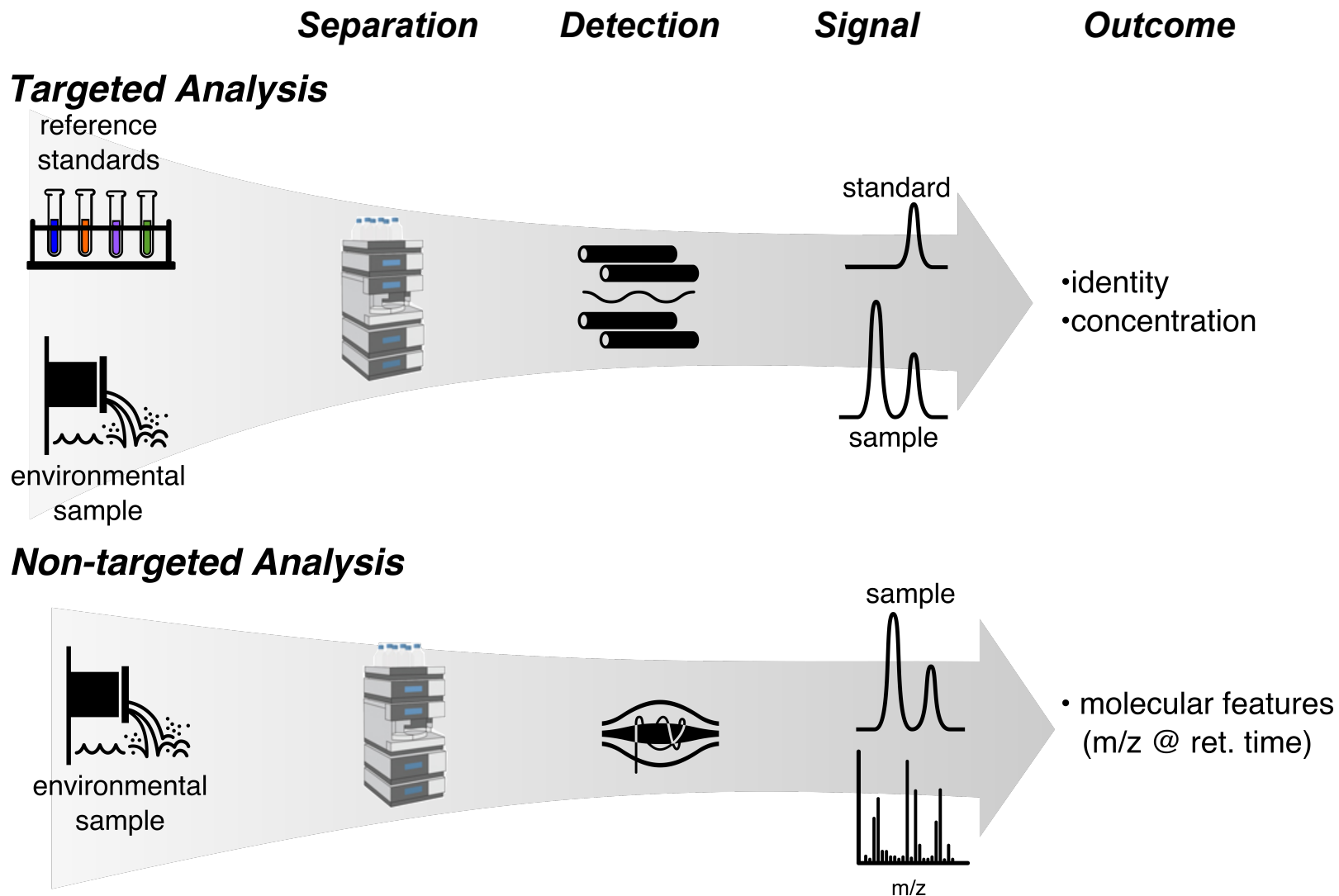
Which organic pollutants occur in environmental waters?



- Chemical space is vast. How can we assess which chemicals in commerce are important as emerging pollutants in the aquatic environment?
- Chemical use, production, and regulation lists are incomplete.
- (Bio)transformation makes prioritization more difficult and compound identification challenging.



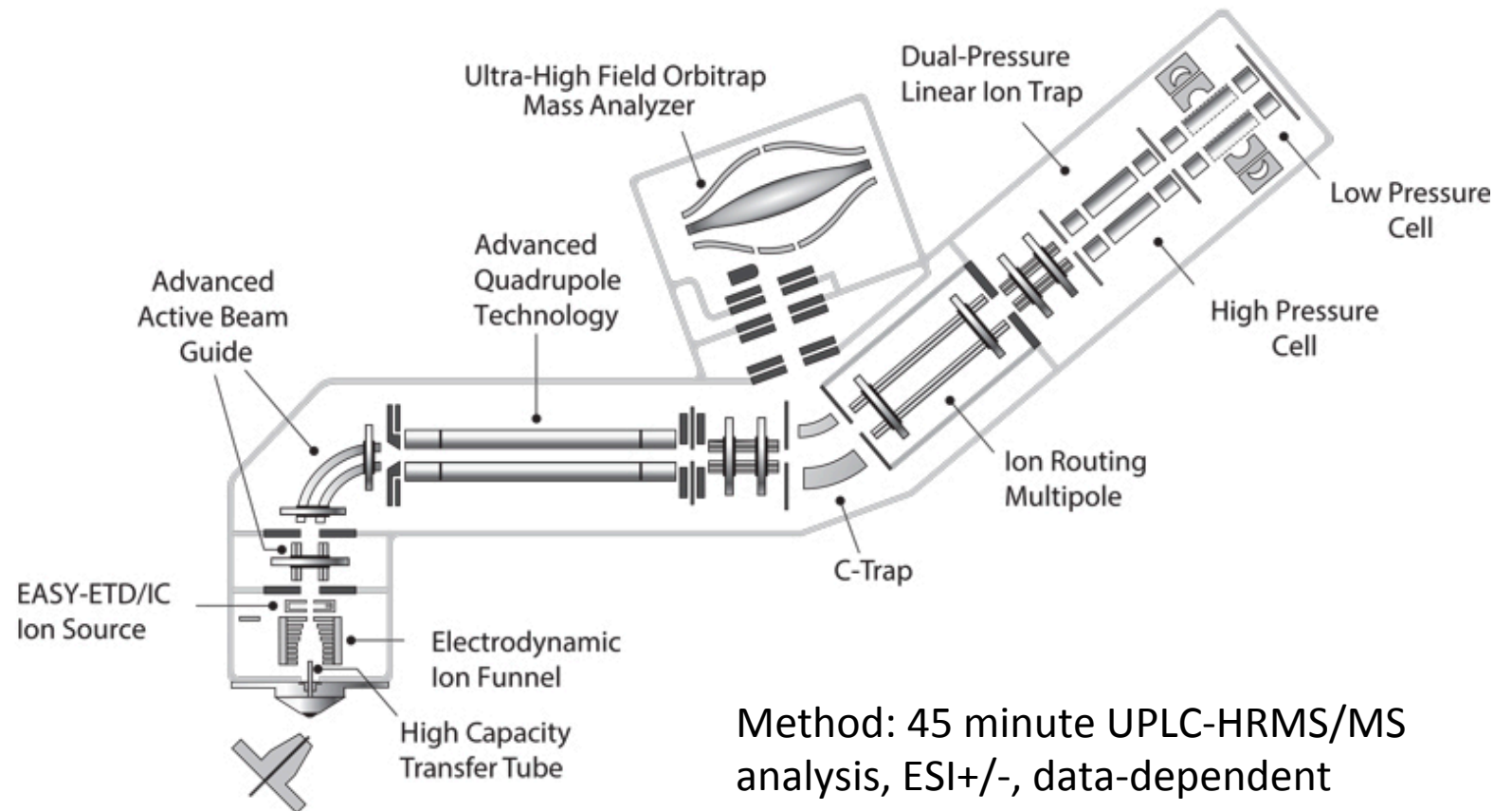
Targeted vs. Non-targeted analysis



Ultra-high resolution mass spectrometry for non-targeted analysis



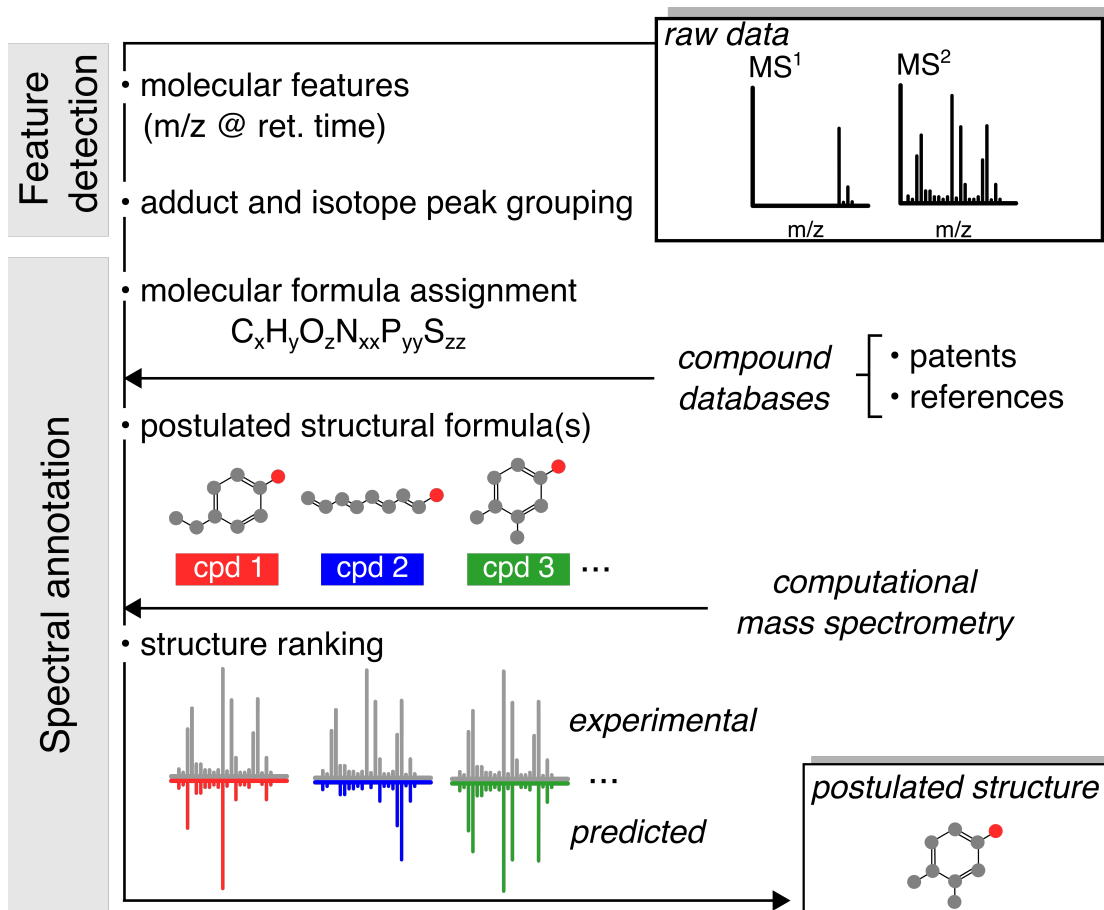
- Orbitrap Fusion Lumos mass spectrometer
- Critical resolution (500,000) and mass accuracy (< 1 ppm)
- Ultra-fast data-dependent MS/MS maximizes data acquisition rate
- MS³ capability for structural characterization
- Ion funnel gives maximum sensitivity



Method: 45 minute UPLC-HRMS/MS analysis, ESI+/-, data-dependent acquisition, internal mass calibration

Data analysis: The hard part!

Overall non-targeted analysis workflow:

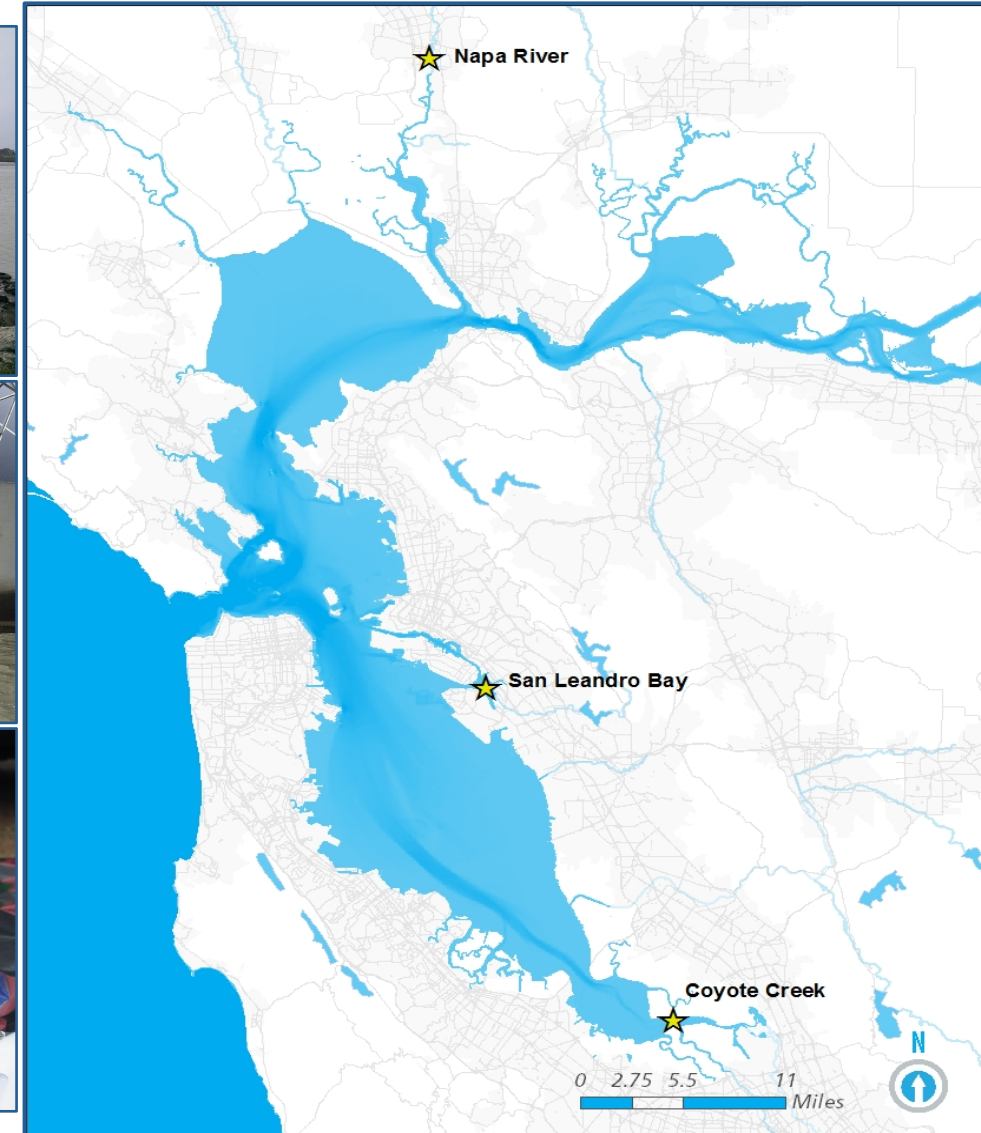


Objectives

- Utilize high-resolution mass spectrometry strategies to identify non-targeted polar organic pollutants in San Francisco Bay waters.
- Assess the performance of passive sampling vs. grab sampling strategies for non-targeted analysis of organic pollutants in Bay waters.
- Examine differences in organic pollutant occurrence and abundance among Bay waters with various pollutant sources.
- Perform reconnaissance of emerging contaminant occurrence in drinking water sources within three watersheds of North Carolina.

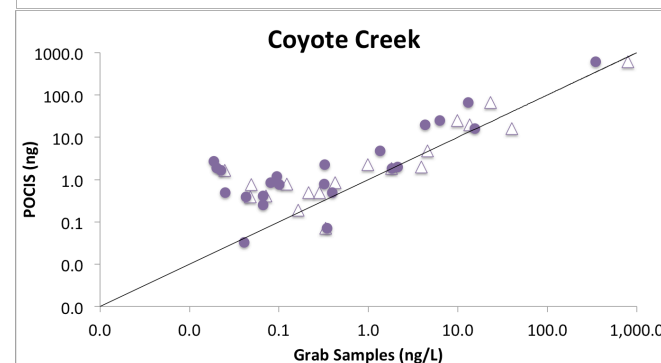
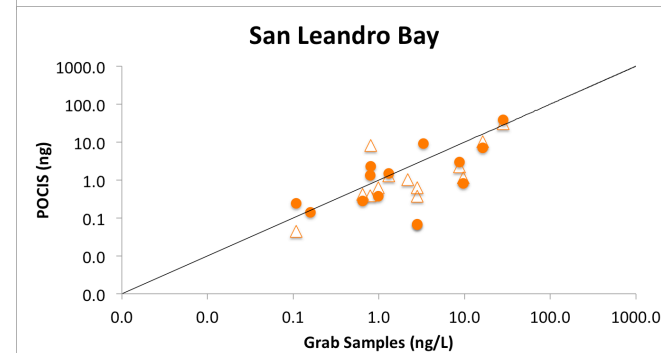
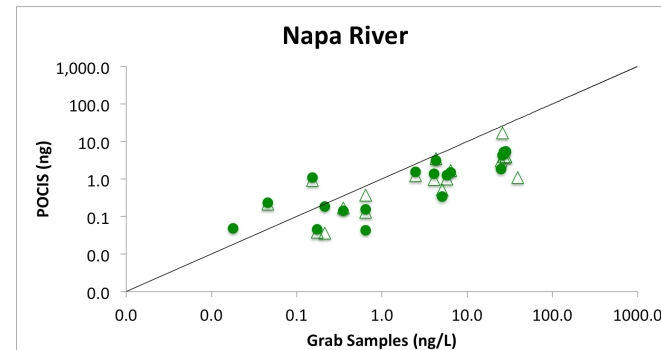
Emerging pollutants in SF Bay waters

- Ambient Bay sample collection:
 - Three sites were sampled: San Leandro Bay (March 2016), Napa River (April 2016), and Coyote Creek (Aug/Sept. 2016)
 - POCIS were deployed for one month at each site.
 - Grab samples (4L volume, one collected in triplicate) were taken at sites on POCIS deployment & retrieval.
 - Field blanks collected for POCIS and grab samples.
- Four WWTP effluent grab samples were collected. Sampling sites were located near the San Leandro Bay and Coyote Creek sites



Target Analyte Quantitation

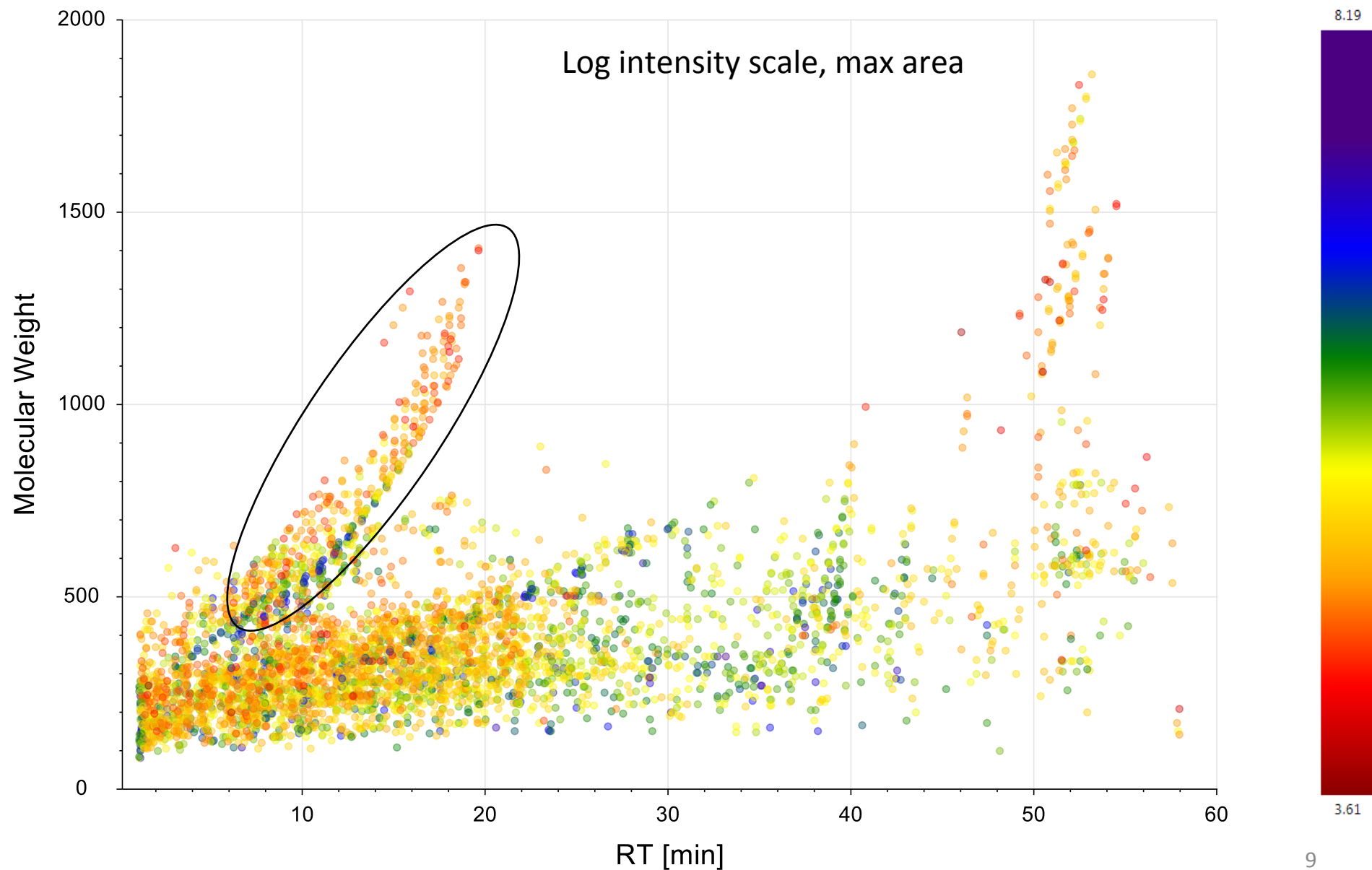
Concentrations in ng/L	Detection Limit	Napa River Deploy	Napa River Retrieval	San Leandro Bay Field Blank	San Leandro Bay Deploy	San Leandro Bay Retrieval	Coyote Creek Deploy	Coyote Creek Retrieval	WWTP Site A	WWTP Site B	WWTP Site C	WWTP Site D	WWTP Site D Field Blank
Agrochemicals:													
Allethrin	1.2				1.33 ± 0.13								
Atrazine	0.06		1.10 ± 0.072									0.296	
Azoxystrobin	0.6	3.09	3.51 ± 0.28								0.68 ± 0.29	3.30	
Benomyl	0.06								23.3				
Carbaryl	0.6	5.33	3.87 ± 0.27			0.628 ± 0.074	0.07						
Carbendazim	0.06	1.39	0.964	0.884 ± 0.38	2.97 ± 0.74	2.21 ± 0.28	6.29 ± 0.14	9.82 ± 0.15	86.6	39.2	40.5 ± 2.1	75.0	
Deet	0.6	1.82	2.98 ± 0.033	0.875 ± 0.37	7.13 ± 0.84	10.4 ± 1.8	4.31 ± 0.43	13.6 ± 0.84	264	61.3	65.0 ± 0.58	13.1	
Fluoxastrobin	0.06	1.10	0.913 ± 0.057	1.70 ± 0.28			0.40	0.29 ± 0.19		0.13	0.14		1.73
Fluridone	0.6	1.52	1.21 ± 0.019				1.83 ± 0.074	1.81 ± 0.20	1.56		3.30 ± 0.18	6.13	
Imazapyr	0.6								1.10				
Metalaxyl	0.06						0.07				0.17		
Prometon	0.06	0.34	0.512 ± 0.012	0.494 ± 0.019	1.47 ± 0.030	1.29 ± 0.074	0.319 ± 0.017	0.12 ± 0.12		0.61	0.42 ± 0.079	5.40	
Simazine	0.6	5.41	3.96 ± 0.20			0.63 ± 0.074						0.98	
Sulfapyridine	0.6						1.36 ± 0.71	4.59 ± 1.1	50.4	49.5	144 ± 4.9	126	
Tertbutylazin-desethyl	0.6	5.41	3.95 ± 0.20									0.979	
Propiconazole	0.6	0.14		3.03 ± 0.331	2.28 ± 0.12	8.14 ± 0.54						4.05	2.38
Pharmaceuticals:													
Carbamazepine	0.6	1.27	1.00 ± 0.11		0.822 ± 0.10	1.16 ± 0.067	13.1 ± 0.12	23.1 ± 1.1	107	125	101 ± 2.0	128	
Cetirizine	0.6	1.50	1.70 ± 0.24			1.03 ± 0.40	15.5 ± 0.41	39.9 ± 1.3	241	440	475 ± 24	454	
cis-Diltiazem	0.06	0.19		0.132 ± 0.007			0.33	0.98 ± 1.3		21.1	46.7 ± 4.1	45.0	
Citalopram	0.06	0.045		0.180 ± 0.014			0.095 ± 0.10			51.4	58.0 ± 0.92		
Dextromethorphan	0.06	0.02								18.3	23.2 ± 0.78		
Diphenhydramine	0.06	0.048		0.086 ± 0.009					0.12	18.8	34.8 ± 3.2	0.508	
Genistein	1.2				9.15 ± 0.11								
Irbesartan	0.6	0.04					2.11 ± 0.21	3.92 ± 0.98	26.3	24.1	70.2 ± 0.31	64.1	
Pramoxine	0.06	0.23	0.215 ± 0.016	0.543 ± 0.024				0.21 ± 0.32	3.68	6.58	0.40 ± 0.32	0.092	
Propanolol	0.06	0.29	0.179 ± 0.013	0.51 ± 0.029						16.4		0.093	
Rosuvastatin	0.6								49.1		1.65 ± 0.41	5.94	
Trimethoprim	0.06	0.16	0.131					0.43	41.0	3.81	5.67 ± 0.52	9.49	
Verapamil	0.6	0.10							7.05		7.72 ± 1.0	5.27	
Benzotriazole	0.06	4.28	16.9 ± 1.6	0.395 ± 0.021	38.1 ± 1.7	30.7 ± 3.7	346 ± 36	792 ± 9.4	1252	701	606 ± 12	1443	



- A variety of agrochemicals and pharmaceutical compounds were detected in WWTP effluents and Bay waters at typically ppt levels.
- Benzotriazole was the most abundant targeted micropollutant in Bay water (Coyote Creek), consistent with high levels in WWTP effluent.
- Target analyte levels in POCIS extracts generally correlated with water concentrations (grab samples) for all sites.

Non-targeted analysis: Data set characteristics

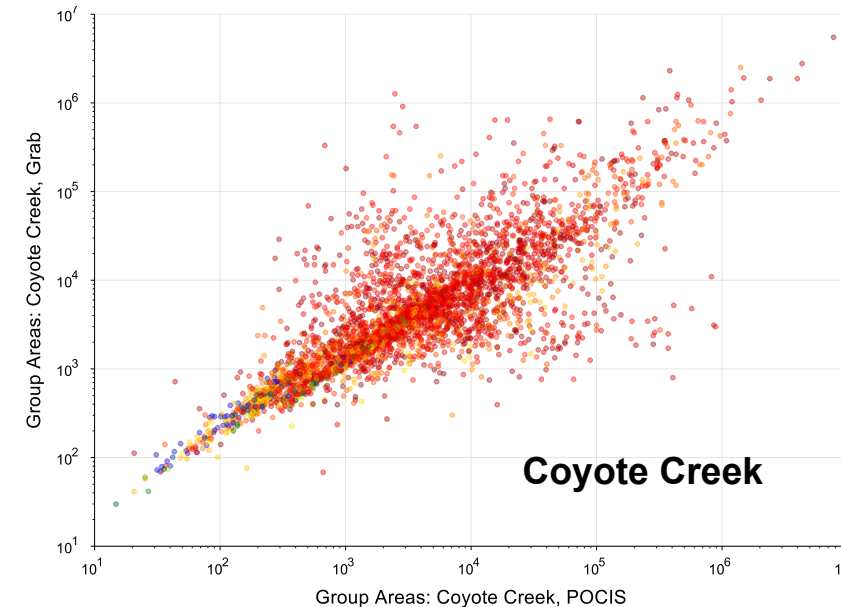
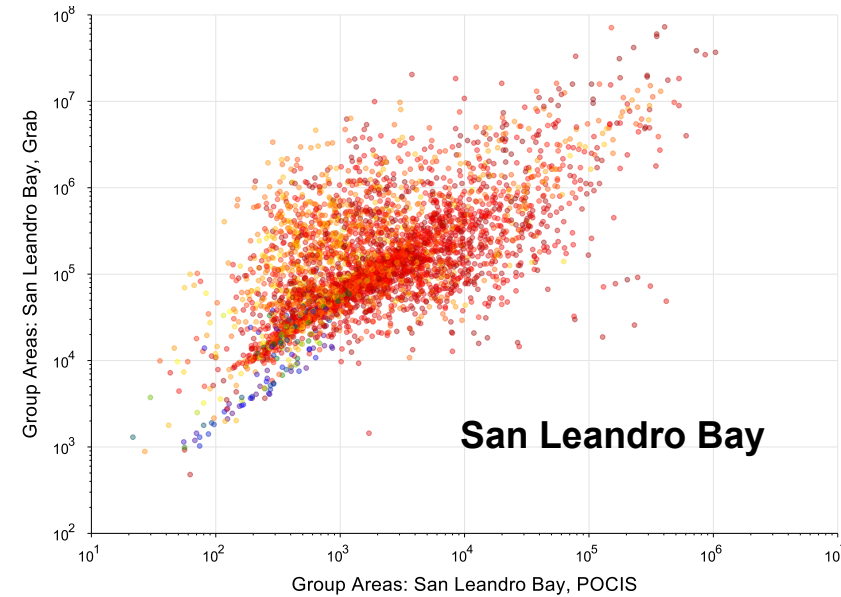
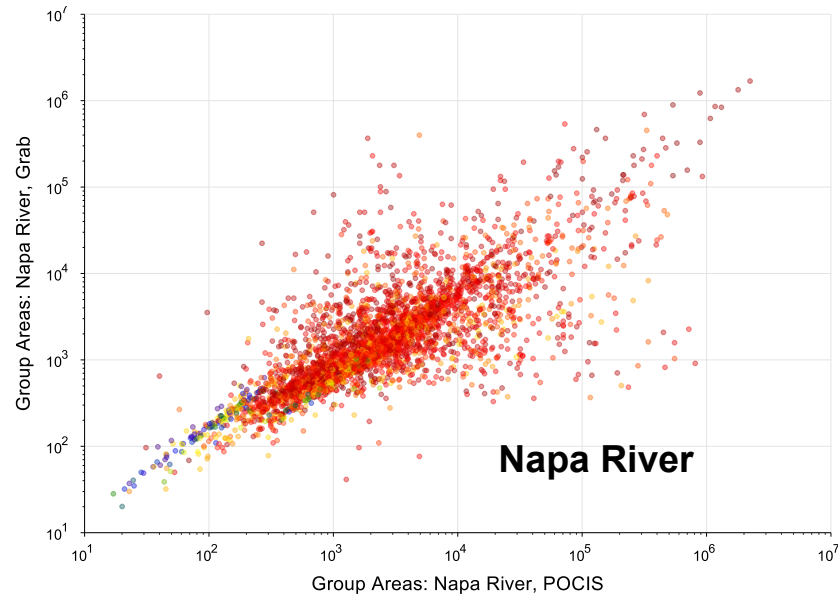
Total # compounds: **4965**
Not on target list: **4630**



Non-targeted analysis data overview: POCIS vs. Grab samples

How well do POCIS extract intensities correlate with intensities of compounds in grab samples?

- High MW, low abundance compounds correlate well at each location.
- Poor correlation is observed for higher abundance compounds in all locations.
- San Leandro Bay POCIS data underpredicts abundance in grab samples

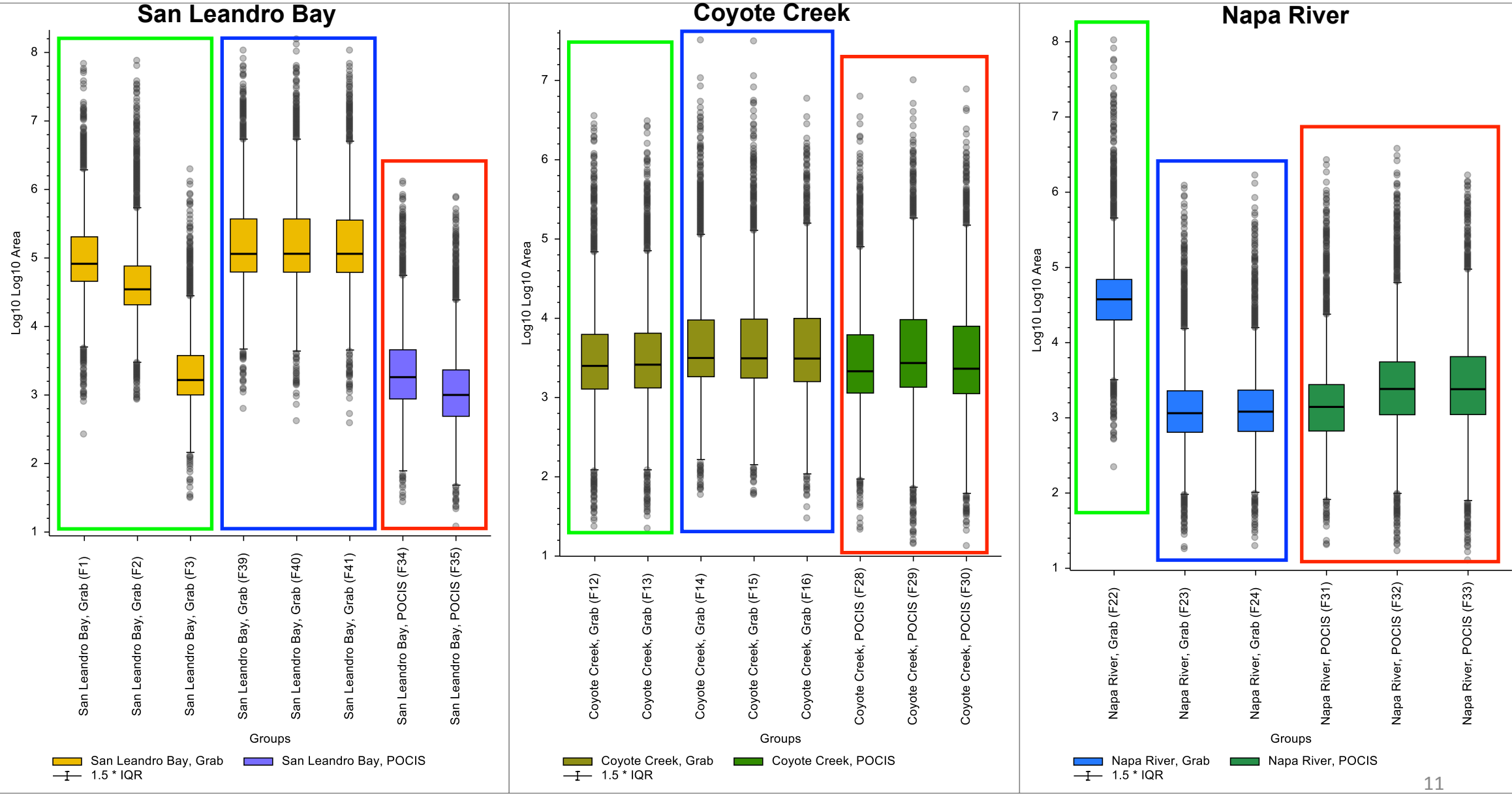


Non-targeted analysis data overview: POCIS and grab sample compound abundance by site

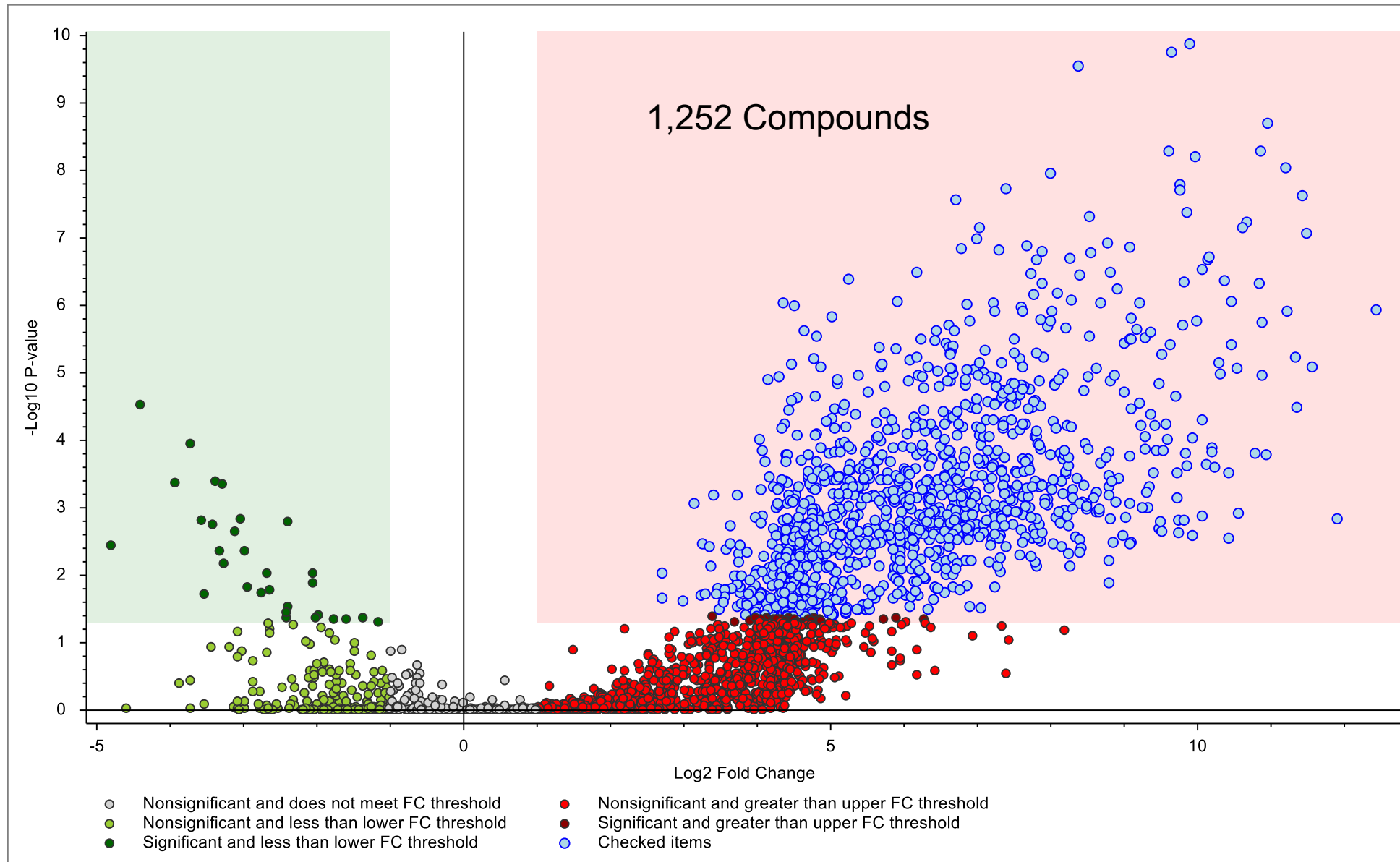
Deployment

Retrieval

POCIS



Differential analysis: Relative abundance of compounds in San Leandro Bay vs. WWTP Effluent (average)



Identifying compounds in San Leandro Bay water:

- Big picture: SLB is extremely complex: Higher pollutant burden than wastewater effluent!
- Large number (> 50) high confidence MS/MS library hits from mzCloud spectral library.
- Occurrence of many polyethoxylated compounds indicates untreated contaminant source.
- Highest abundance compounds identified are fungicide myclobutanil and several polymer/rubber additives.
- Pharmaceuticals and illicit drugs are also identified with high confidence.

Compound Discoverer 2.1.0.326

File Reporting Libraries View Window Help

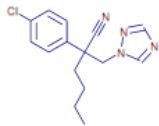
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Compounds Compounds per File Merged Features Features mzVault Results mzCloud Results ChemSpider Results Mass List Search Results Input Files

	Checked	Name	Formula	Annotation Sc	Molecular Weight	RT [min]	Area (Max.)	# MS2	# ChemSpider Results	# mzCloud Results	mzCloud Best Match
1	<input checked="" type="checkbox"/>	Myclobutanil	C15 H17 Cl N4	■■■■■	288.11446	28.935	57126323	6	14	1	81.4
2	<input checked="" type="checkbox"/>	N,N'-Diphenylguanidine	C13 H13 N3	■■■■■	211.11117	7.265	54003060	23	50	2	89.9
3	<input checked="" type="checkbox"/>	Caprolactam	C6 H11 N O	■■■■■	113.08419	3.350	52884350	28	145	1	77.6
4	<input checked="" type="checkbox"/>	PEG (12EO)		■■■■■	563.35120	10.912	19001426	1	0	1	87.9
5	<input checked="" type="checkbox"/>	PEG (12EO)		■■■■■	563.35140	10.833	19001426.067364939	0	0	1	87.9
6	<input checked="" type="checkbox"/>	PEG (13EO)		■■■■■	607.37757	11.770	16711576	1	1	1	85.1
7	<input checked="" type="checkbox"/>	PPG (10EO)		■■■■■	620.41070	27.612	6870340	1	1	1	75.8
8	<input checked="" type="checkbox"/>	Benzoyllecgonine	C16 H19 N O4	■■■■■	289.13157	7.910	5410580	10	43	2	81.2
9	<input checked="" type="checkbox"/>	Cocaine	C17 H21 N O4	■■■■■	303.14726	11.853	3688306	5	63	1	84.0
10	<input checked="" type="checkbox"/>	N~5~-(Diaminomethylene)-L-ornith	C18 H36 N6 O4	■■■■■	400.27971	36.820	3445412	1	1	1	77.1
11	<input checked="" type="checkbox"/>	Paracetamol	C8 H9 N O2	■■■■■	151.06346	2.566	3181711	3	293	4	94.3
12	<input checked="" type="checkbox"/>	8-Hydroxyquinoline	C9 H7 N O	■■■■■	145.05285	4.207	2761085	9	91	1	77.3
13	<input checked="" type="checkbox"/>	Nobiletin	C21 H22 O8	■■■■■	402.13173	27.164	2615802	4	28	1	88.7
14	<input checked="" type="checkbox"/>	6-Methoxyquinoline	C10 H9 N O	■■■■■	159.06853	2.215	1883138	17	225	1	80.8
15	<input checked="" type="checkbox"/>	Benzothiazole	C7 H5 N S	■■■■■	135.01421	12.683	1765156	1	17	1	94.6
16	<input checked="" type="checkbox"/>	2-Hydroxysimazine	C7 H13 N5 O	■■■■■	183.11235	3.950	1763410	4	18	1	94.4
17	<input checked="" type="checkbox"/>	Cotinine	C10 H12 N2 O	■■■■■	176.09511	1.644	1317652	14	222	2	95.2
18	<input checked="" type="checkbox"/>	PEG (14EO)		■■■■■	651.40422	13.564	1006321	1	0	1	83.9
19	<input checked="" type="checkbox"/>	δ-Valerolactam	C5 H9 N O	■■■■■	99.06848	2.257	997237	1	86	3	83.5
20	<input checked="" type="checkbox"/>	N~5~-(Diaminomethylene)-L-ornith	C18 H36 N6 O4	■■■■■	400.28026	38.099	852226	1	1	1	76.5
21	<input checked="" type="checkbox"/>	2-[[Dimethylamino)methylidene]ind	C12 H13 N O	■■■■■	187.09985	3.390	782328	2	203	1	75.9
22	<input checked="" type="checkbox"/>	Caprolactam		■■■■■	113.08253	3.349	739621	1	0	1	77.6
23	<input checked="" type="checkbox"/>	Isoquinoline	C9 H7 N	■■■■■	129.05784	2.644	720716	3	23	1	83.4
24	<input checked="" type="checkbox"/>	PPG (9EO)		■■■■■	562.36932	35.702	426723	2	0	1	75.9
25	<input checked="" type="checkbox"/>	1-(1,3,3-Trimethyl-2,3-dihydro-1H-ir	C14 H17 N O	■■■■■	215.13080	6.820	279968	2	135	1	83.2

Hide Related Tables

Structure Proposals Compounds per File Predicted Compositions Merged Features Matched Patterns mzVault Results mzCloud Results ChemSpider Results Mass List Search Results

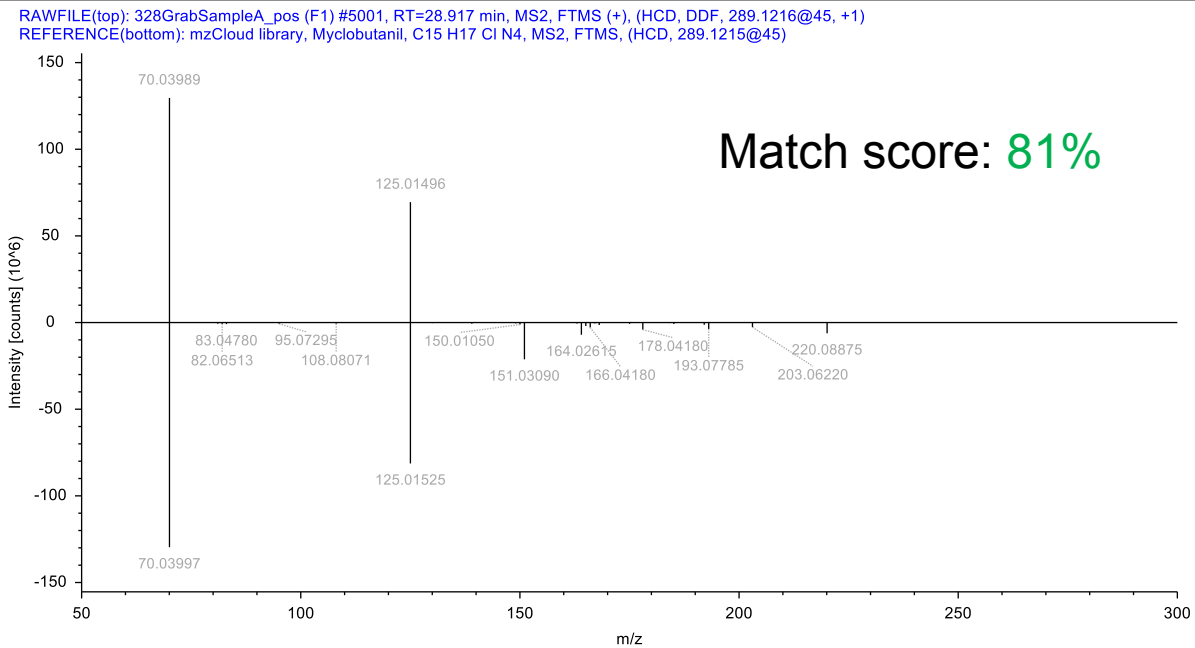
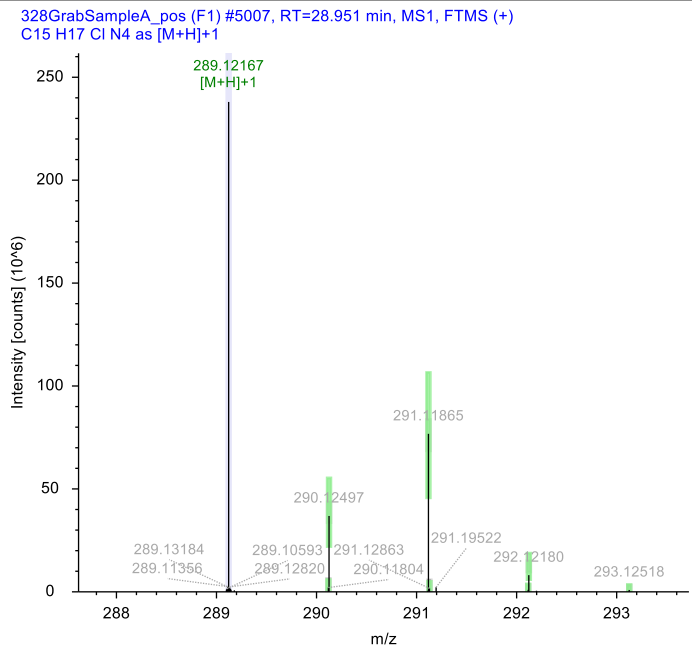
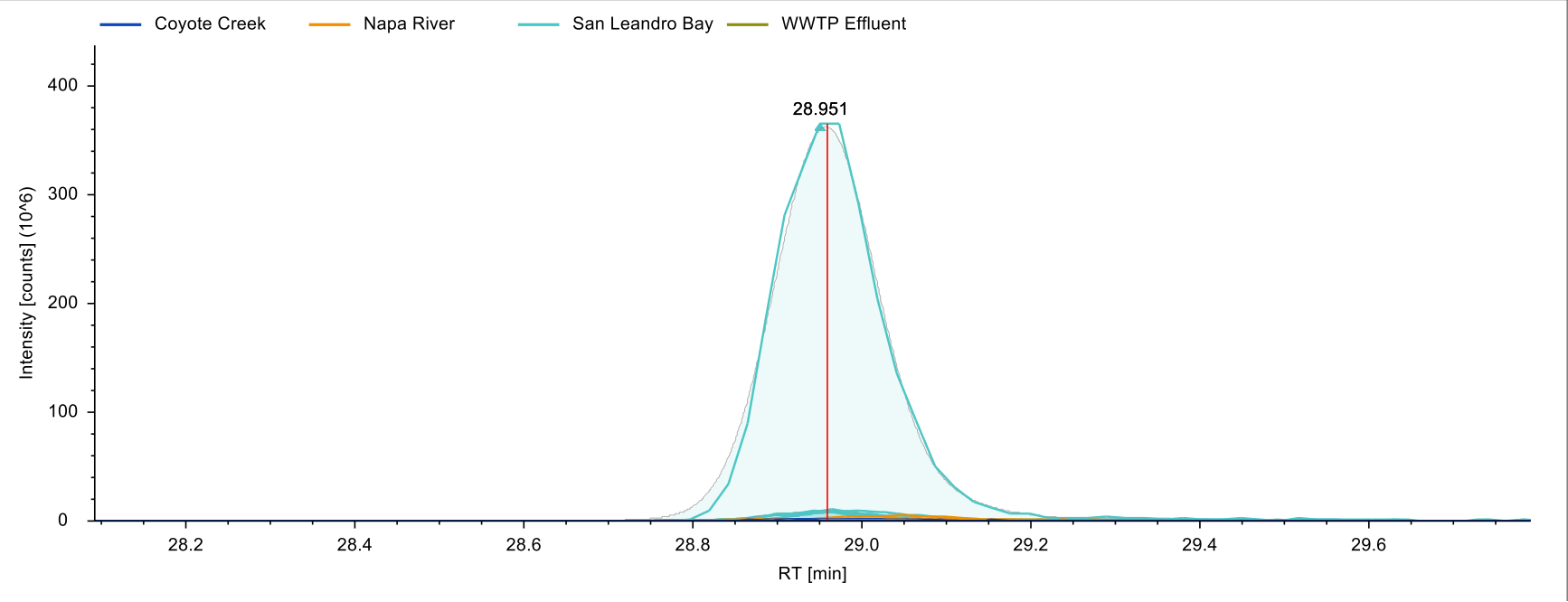
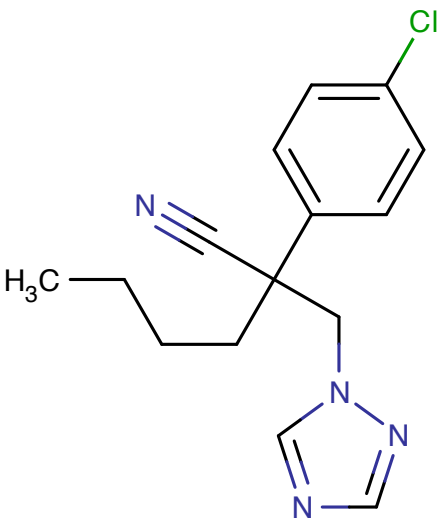
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Show Related Tables

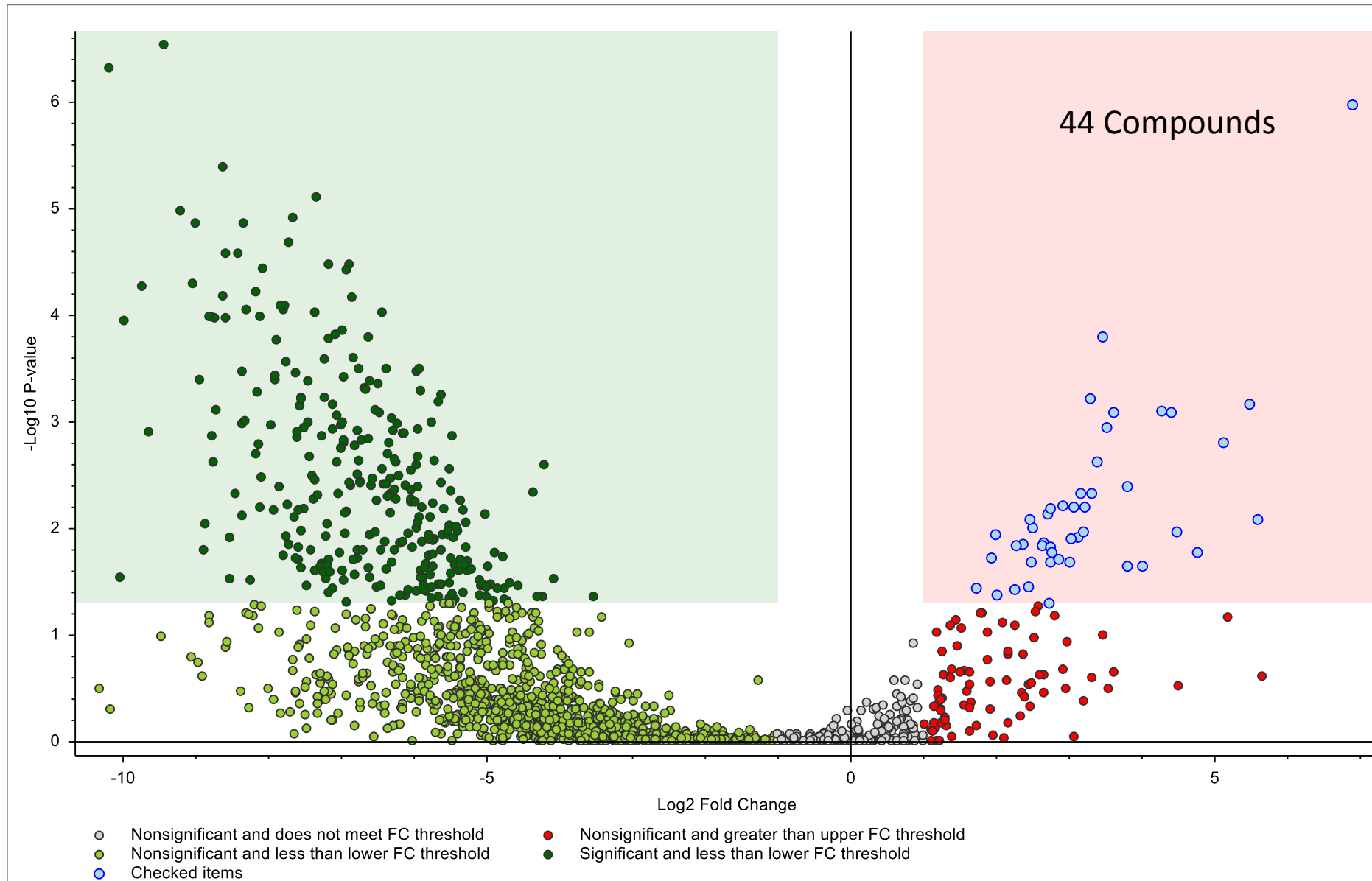
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Myclobutanil: Conazole fungicide used to control fungal infections in table & wine grapes (primarily in California). Also used for cannabis cultivation.

<http://www.toxipedia.org/display/toxipedia/Myclobutanil>



Differential analysis: Relative abundance of compounds in Napa River vs. WWTP Effluent (average)



Identifying compounds in Napa River water:

- Far fewer compounds had elevated levels in Napa River water relative to WWTP effluent.
- Only one compound (2-hydroxysimazine) matched with high confidence to library spectra.
- Highly uncertain (mass-only) tentative identifications of other compounds indicates many natural products.
- No indication of significant wastewater pollutant sources in the Napa River.
- Several candidates had MS/MS spectra consistent with agrochemicals and commercial chemical transformation products.

Compound Discoverer 2.1.0.326

File Reporting Libraries View Window Help

Start Page x SFEL_NonTarget_20170322 x Job Queue x SFEL_2017_0328a x

Compounds Compounds per File Merged Features Features mzVault Results mzCloud Results ChemSpider Results Mass List Search Results Input Files

	Checked	Name	Formula	Annotation Sc	Molecular Weight	RT [min]	Area (Max.)	# MS2	# ChemSpider Results	# mzCloud Results	mzCloud Best Match
1	<input checked="" type="checkbox"/>	1,9-Dihydroxy-3,6,11,14-tetraphenyl	C40 H26 O5	■ ■ ■ ■ ■	586.17842	28.700	19590570	7	3	0	
2	<input checked="" type="checkbox"/>	2-Amino-5,6,7,8-tetrahydro-4(1H)-q	C8 H11 N3 O	■ ■ ■ ■ ■	165.09052	2.054	13385868	5	93	0	
3	<input checked="" type="checkbox"/>	l-Phe-l-Phe	C18 H20 N2 O3	■ ■ ■ ■ ■	312.14813	29.180	11792074	2	66	0	
4	<input checked="" type="checkbox"/>	Butyl 4-[(4-nitrobenzoyl)amino]benz	C18 H18 N2 O5	■ ■ ■ ■ ■	342.12213	23.676	5515307	4	22	0	
5	<input checked="" type="checkbox"/>	1-carboxy-3-hydroxyadamantane	C11 H16 O3	■ ■ ■ ■ ■	196.11015	8.367	4966869	12	232	0	
6	<input checked="" type="checkbox"/>	Sulfolane	C4 H8 O2 S	■ ■ ■ ■ ■	120.02458	1.736	4862130	1	33	0	
7	<input checked="" type="checkbox"/>	2-Methyl-3-phenyl-N,N-dipropylpro	C16 H25 N O	■ ■ ■ ■ ■	247.19427	3.711	4853615	4	79	0	
8	<input checked="" type="checkbox"/>	1-carboxy-3-hydroxyadamantane	C11 H16 O3	■ ■ ■ ■ ■	196.10969	8.354	4083859	2	232	0	
9	<input checked="" type="checkbox"/>	(+)-Abscisic acid	C15 H20 O4	■ ■ ■ ■ ■	264.13651	15.138	2704250	4	154	0	
10	<input checked="" type="checkbox"/>	Cinnamic acid	C9 H8 O2	■ ■ ■ ■ ■	148.05238	23.600	2454758	2	101	0	
11	<input checked="" type="checkbox"/>	3-[5-[[3-(2-carboxyethyl)-5-[[3-(2-ca	C35 H38 N4 O10	■ ■ ■ ■ ■	674.25945	16.979	2366026	3	3	0	
12	<input checked="" type="checkbox"/>	Lacosamide	C13 H18 N2 O3	■ ■ ■ ■ ■	250.13226	4.729	2331269	3	125	0	
13	<input checked="" type="checkbox"/>	Ancymidol	C15 H16 N2 O2	■ ■ ■ ■ ■	256.12144	17.140	2301205	4	136	1	57.0
14	<input checked="" type="checkbox"/>	1,9-Dihydroxy-3,6,11,14-tetraphenyl	C40 H26 O5	■ ■ ■ ■ ■	586.17674	28.778	2202900	1	3	0	
15	<input checked="" type="checkbox"/>	Methoxyfenozide	C22 H28 N2 O3	■ ■ ■ ■ ■	368.21060	29.181	1961423	2	34	0	
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17	<input checked="" type="checkbox"/>	2-Hydroxysimazine	C7 H13 N5 O	■ ■ ■ ■ ■	183.11235	3.950	1763410	4	18	1	94.4
18	<input checked="" type="checkbox"/>	6,7-Dimethoxy-2,2-dimethylchrome	C13 H16 O3	■ ■ ■ ■ ■	220.11008	14.018	1711739	5	281	0	
19	<input checked="" type="checkbox"/>	Tolmetin	C15 H15 N O3	■ ■ ■ ■ ■	257.10520	17.134	1649184	6	199	0	
20	<input checked="" type="checkbox"/>	2,2,2-Trifluoro-N-[3-methyl-1-(2-ph	C22 H25 F3 N2 O	■ ■ ■ ■ ■	390.19147	29.137	1378679	3	1	0	
21	<input checked="" type="checkbox"/>	Oxadixyl	C14 H18 N2 O4	■ ■ ■ ■ ■	278.12685	5.874	1240518	13	72	0	
22	<input checked="" type="checkbox"/>	Methyl 3,5-di-tert-butyl-4-hydroxyb	C16 H24 O3	■ ■ ■ ■ ■	264.17314	34.758	1237294	1	80	1	53.0
23	<input checked="" type="checkbox"/>	(2E)-2-(1,3-Benzothiazol-2-yl)-3-[9-r	C26 H18 N4 O2 S	■ ■ ■ ■ ■	450.11500	3.948	1230553	6	7	0	
24	<input checked="" type="checkbox"/>	Ethyl 6-nitro-2-oxo-4-phenyl-1,2-dil	C18 H14 N2 O5	■ ■ ■ ■ ■	338.09080	20.873	1150352	4	40	0	
25	<input checked="" type="checkbox"/>	3-Ethyl 1-(2-methyl-2-propanyl) 3-b	C20 H29 N O4	■ ■ ■ ■ ■	347.21024	35.125	1111333	4	13	0	

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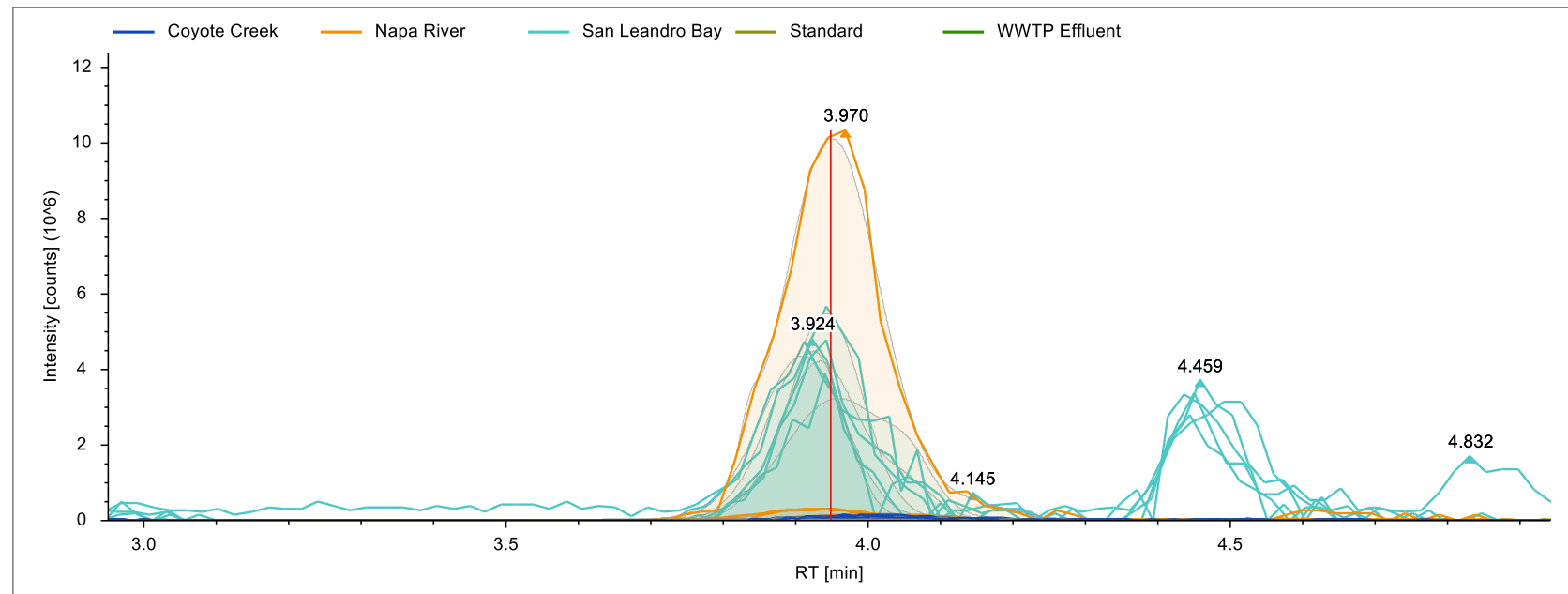
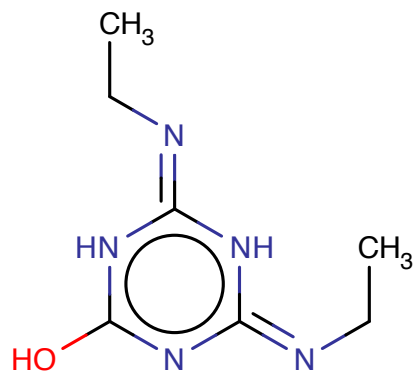
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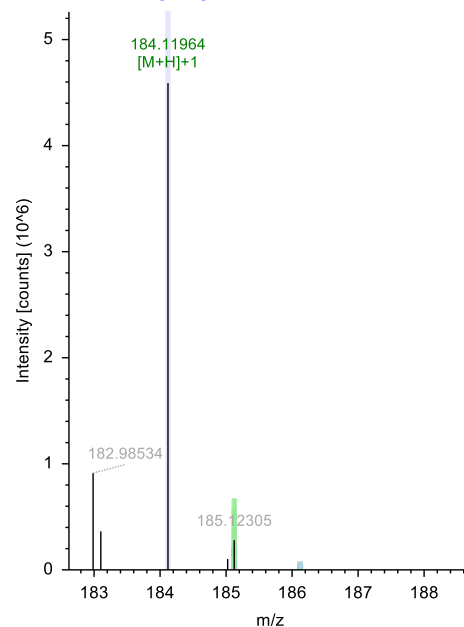
16

2-Hydroxysimazine:

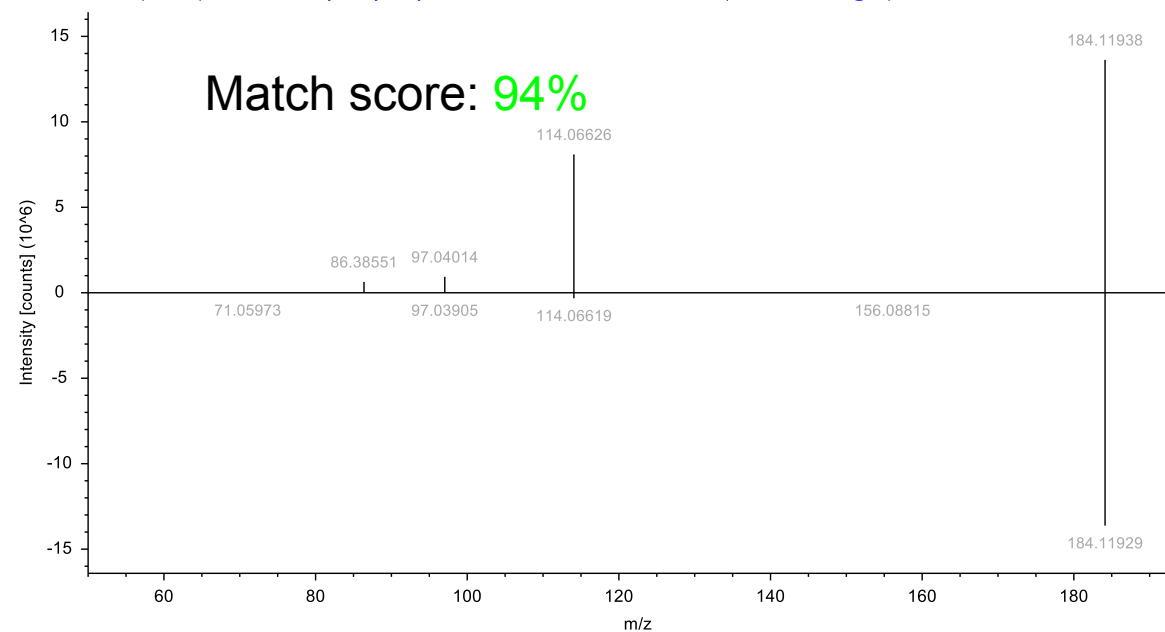
Transformation product of the widely-used triazine herbicide simazine (broadleaf weed and grass killer).



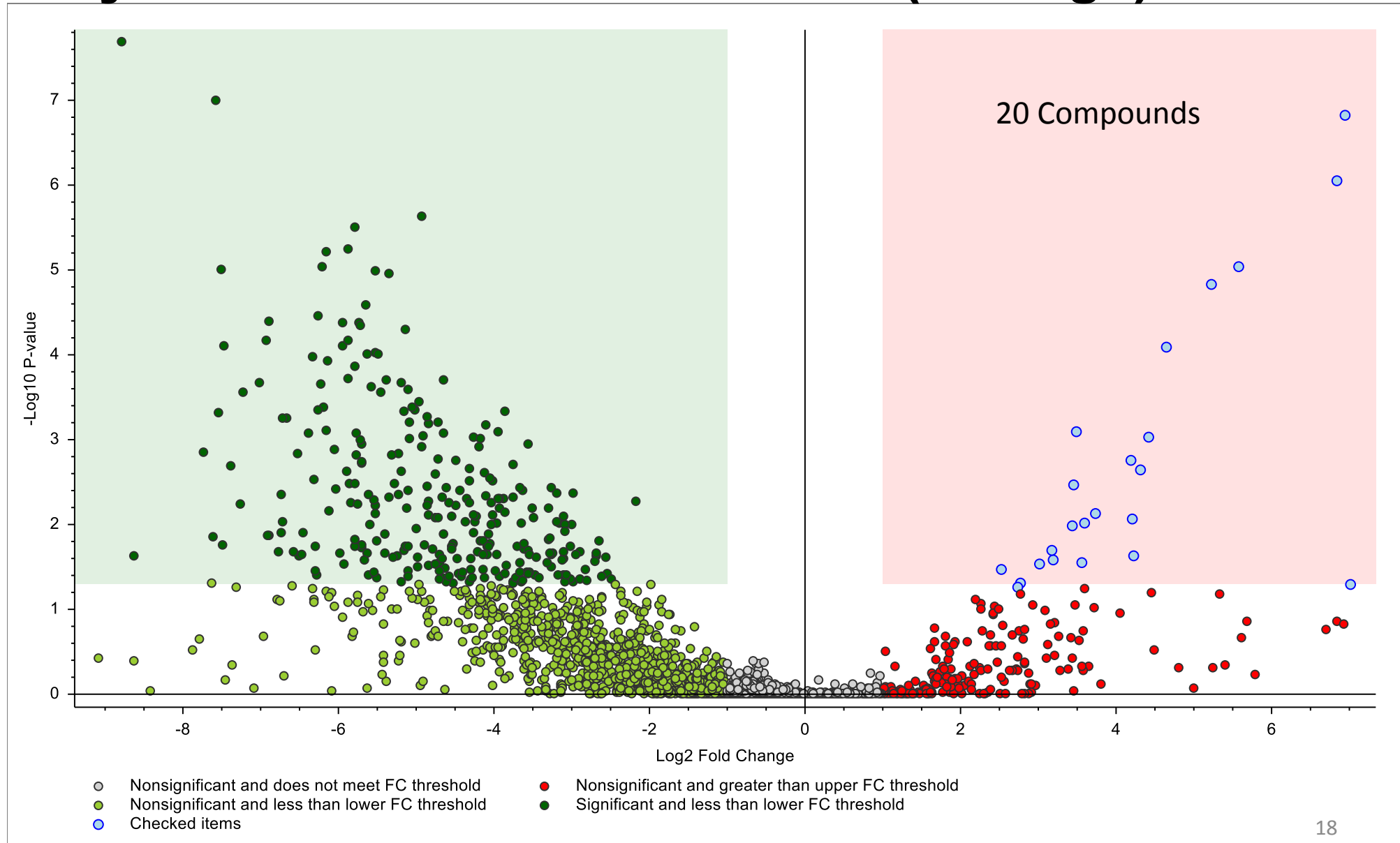
NapaRiverDeployGrab_pos (F22) #489, RT=3.870 min, MS1, C7 H13 N5 O as [M+H]⁺1



RAWFILE(top): NapaRiverDeployGrab_pos (F22) #490, RT=3.877 min, MS2, FTMS (+), (HCD, DDF, 184.1196@45, +1)
REFERENCE(bottom): mzCloud library, 2-Hydroxysimazine, C7 H13 N5 O, MS2, FTMS, (HCD, 184.1193@30)



Differential analysis: Relative abundance of compounds in Coyote Creek vs. WWTP Effluent (average)



Identifying compounds in Coyote Creek water:

- Few unique compounds in Coyote Creek.
- Most detected compounds are also found in high abundance in WWTP effluent (Coyote Creek resembles diluted effluent).
- No high confidence identifications from Spectral library.
- Several low-confidence spectral library matches can be examined.

Compound Discoverer 2.1.0.323

File Reporting Libraries View Window Help

Start Page x SFEI_2017_0324 x

Compounds Compounds per File Merged Features Features mzVault Results mzCloud Results ChemSpider Results Mass List Search Results Input Files

	Checked	Name	Formula	Predicted Compositions* mzCloud Search mzVault Search ChemSpider Search MassList Match	Molecular Weight	RT [min]	# MS2	Area (Max.)	mzCloud Best Match	# mzCloud Results	# ChemSpider Results
1	<input checked="" type="checkbox"/>	2-Methyl-2-propanyl 4-(4-hydroxyb	C14 H27 N O3	■ ■ ■ ■ ■	257.19905	33.965	4	4121099		0	31
2	<input checked="" type="checkbox"/>	5-(3-Bromo-4-methoxyphenyl)-1H-1	C8 H7 Br N4 O	■ ■ ■ ■ ■	253.97973	1.134	1	2071379		0	6
3	<input checked="" type="checkbox"/>	Methylprednisolone	C22 H30 O5	■ ■ ■ ■ ■	374.20927	33.689	7	1192510		0	20
4	<input checked="" type="checkbox"/>			■ ■ ■ ■ ■	139.99927	1.140	5	872810		0	0
5	<input checked="" type="checkbox"/>	(6beta,7alpha)-7,11,12-Trihydroxy-6,	C20 H26 O5	■ ■ ■ ■ ■	346.17801	30.548	2	839555		0	23
6	<input checked="" type="checkbox"/>	4-Butoxy-3-ethoxybenzoic acid	C13 H18 O4	■ ■ ■ ■ ■	238.12055	16.266	3	734564		0	163
7	<input checked="" type="checkbox"/>	1,1'-hexane-1,6-diylbis(1H-pyrrole-2	C14 H16 N2 O4	■ ■ ■ ■ ■	276.11110	7.263	16	711474		0	68
8	<input checked="" type="checkbox"/>	3,3'-Dimethoxybenzidine	C14 H16 N2 O2	■ ■ ■ ■ ■	244.12116	10.838	2	457741	52.0	1	199
9	<input checked="" type="checkbox"/>	N-(tert-Butoxycarbonyl)-3-methyl-L-	C11 H21 N O4	■ ■ ■ ■ ■	231.14719	6.110	8	414957		0	67
10	<input checked="" type="checkbox"/>	N-(2-Methyl-2-propanyl)-N-[(Z)-(1- <i>c</i>	C10 H14 N2 O2	■ ■ ■ ■ ■	194.10581	1.889	9	255782		0	278
11	<input checked="" type="checkbox"/>	Methylenedioxybenzylpiperazine	C12 H16 N2 O2	■ ■ ■ ■ ■	220.12129	3.402	9	236827		0	237
12	<input checked="" type="checkbox"/>	N-Boc-L-proline	C10 H17 N O4	■ ■ ■ ■ ■	215.11582	3.588	8	225642		0	77
13	<input checked="" type="checkbox"/>	Benalaxyl	C20 H23 N O3	■ ■ ■ ■ ■	325.16774	14.913	8	179097		0	67
14	<input checked="" type="checkbox"/>			■ ■ ■ ■ ■	473.28339	4.606	2	172332		0	0
15	<input checked="" type="checkbox"/>	1-Phenylhexahydropyridazine-3,6-di	C10 H10 N2 O2	■ ■ ■ ■ ■	190.07421	7.636	1	99523	55.5	1	370
16	<input checked="" type="checkbox"/>	Crocin	C20 H24 O4	■ ■ ■ ■ ■	328.16732	26.368	2	94433		0	41
17	<input checked="" type="checkbox"/>	Atropine	C17 H23 N O3	■ ■ ■ ■ ■	289.16790	12.468	4	84052	62.0	3	67
18	<input checked="" type="checkbox"/>	3-(<i>n</i> -methyl- <i>p</i> -((<i>p</i> -nitrophenyl)azo)a	C16 H15 N5 O2	■ ■ ■ ■ ■	309.12264	11.684	7	82655		0	12
19	<input checked="" type="checkbox"/>	3-morpholino-2-(morpholinomethyl)	C12 H21 N3 O2	■ ■ ■ ■ ■	239.16358	6.206	1	54734		0	28
20	<input checked="" type="checkbox"/>	6-Hydroxy-N-[[[2-methyl-2-propany	C11 H21 N O5	■ ■ ■ ■ ■	247.14200	4.392	7	48172		0	10
21	<input checked="" type="checkbox"/>	2-Methyl-2-propanyl 3-(hydroxymet	C11 H18 F3 N O3	■ ■ ■ ■ ■	269.12399	3.592	8	47493		0	2

Hide Related Tables

Structure Proposals Compounds per File Predicted Compositions Merged Features Matched Patterns mzVault Results mzCloud Results ChemSpider Results Mass List Search Results

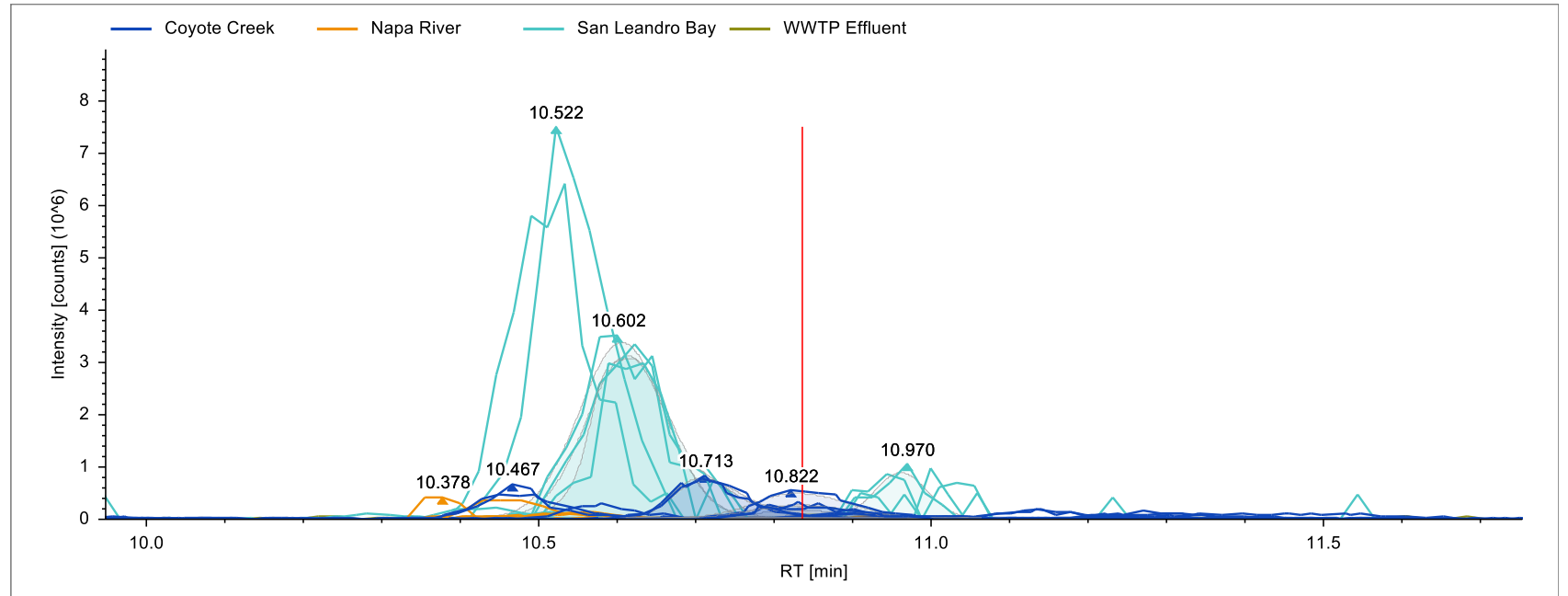
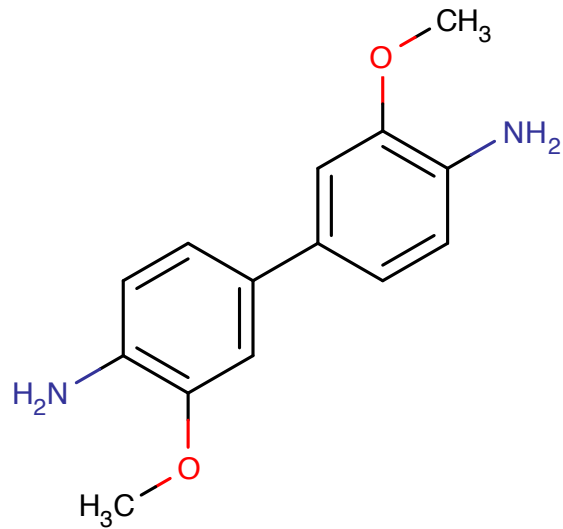
	Checked	Compound	ΔMass [Da]	ΔMass [ppm]	Scan Number	mzCloud ID	Formula	Structure	Molecular Weight	Match	Best Match	Name
1	<input checked="" type="checkbox"/>		0.00002	0.09	1253	1842	C14 H16 N2 O2		244.12118	52.0	59.6	3,3'-Dimethoxybenzidine

Show Related Tables

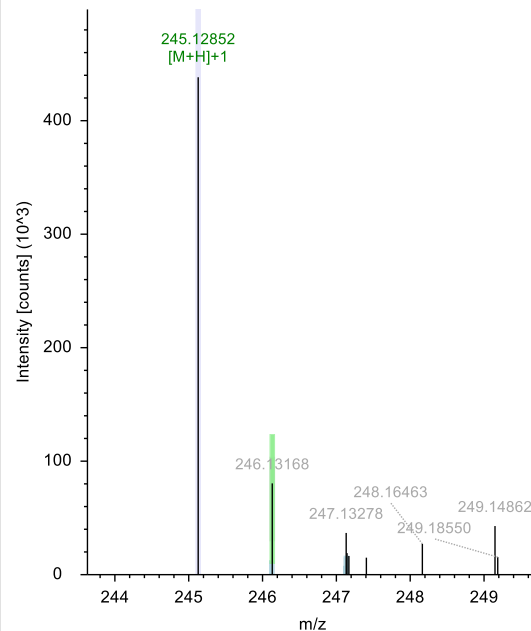
19

3,3'-Dimethoxybenzidine?

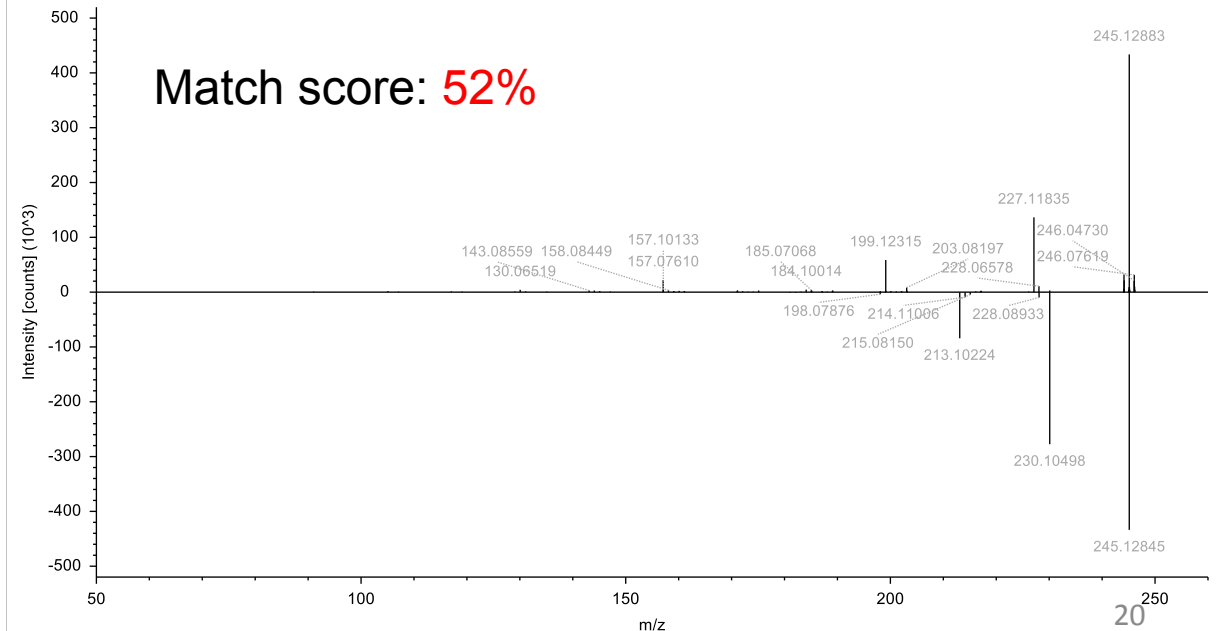
This could be a reductive transformation product of diazobenzene dyes, but the spectral match is relatively poor.



CoyoteCreekRetrievalGrabC_pos (F16) #1261, RT=10.840 min, MS1, F
C14 H16 N2 O2 as [M+H]⁺



RAWFILE(top): CoyoteCreekRetrievalGrabC_pos (F16) #1253, RT=10.759 min, MS2, FTMS (+), (HCD, DDF, 245.1288@45, +1)
REFERENCE(bottom): mzCloud library, 3,3'-Dimethoxybenzidine, C14 H16 N2 O2, MS2, FTMS, (HCD, 245.1285@30)



Match score: **52%**

Can library match be verified by *in silico* fragmentation?

Computational fragment tree analysis by Sirius 3.4 supports the assignment of $C_{14}H_{16}N_2O_2$ as candidate molecular formula...



Can library match be verified by *in silico* fragmentation?

... however, structural fragment matching does not support identity of compound as 3,3'-dimethoxybenzidine.

An alternative identity may be Amidate (Etomidate), an anesthetic/hypnotic compound used in medical procedures. This must be considered a tentative identification.

Sirius 3.4.1 (build 6)

Import Batch Import Load Workspace Save Workspace Compute All Export Results CSI:FingerId Jobs Settings Bug Report About

Experiments Identifications Overview Spectra view Tree view CSI:FingerId

Filter:

586.1784@28.68
ionization [M + H]⁺
parent mass 587.19 Da
1 ms1 spectrum
1 ms2 spectrum ✓

586.1784@28.68 (2)
ionization [M + H]⁺
parent mass 587.19 Da
1 ms1 spectrum
1 ms2 spectrum ✓

165.0905@2.01
ionization [M + H]⁺
parent mass 166.10 Da
1 ms1 spectrum
1 ms2 spectrum ✓

256.1215@17.14
ionization [M + H]⁺
parent mass 257.13 Da
1 ms1 spectrum
1 ms2 spectrum ✓

450.1150@3.86
ionization [M + H]⁺
parent mass 451.12 Da
1 ms1 spectrum
1 ms2 spectrum ✓

264.1731@34.74
ionization [M + H]⁺
parent mass 265.18 Da
1 ms1 spectrum
1 ms2 spectrum ✓

244.1212@10.84
ionization [M + H]⁺
parent mass 245.13 Da
1 ms1 spectrum
1 ms2 spectrum ✓

1 C₁₄H₁₆N₂O₂ + H⁺ Score: 47.306630 ✓
2 C₁₀H₁₉N₃O₂P + H⁺ Score: 6.604772
3 C₆H₁₆N₈O₅ + H⁺ Score: -0.250970
4 C₇H₁₆N₈ + H⁺ Score: -9.065083
5 C₁₁H₁₉CIN₃O + H⁺ Score: -9.715937
6 C₂H₁₉N₉O₅Si + H⁺ Score: -15.118596

XLogP filter: -2.00 8.00

☐ Biocyc ☐ biological ☒ CHEBI ☐ custom ☒ GNPS ☒ HMDB ☐ HSDB ☒ KEGG ☒ KnapSack ☒ Maconda ☒ MeSH ☐ Natural Products ☐ PubChem ☐ PubMed ☒ training set

Amidate NPUKDXFDDZOKR XLogP: 2.874
Substructures:

Databases: [training set](#) [HMDB](#) [CHEBI](#) [ZINC bio](#) [KEGG](#) [MeSH](#) [biological](#) [GNPS](#)

5282 score: e⁻⁴⁸¹³

OVNQNQOVBVQZCE XLogP: 1.116
Substructures:

Databases: [MeSH](#)

6079 score: e⁻⁴⁸¹⁹
N-beta-Naphthylaminomethyl-L-alanine ZYBUKDDPDSFHHK XLogP: 2.593
Substructures:

Databases: [MeSH](#) [biological](#)

7005

Alternative approaches for prioritizing compounds for identification:

- Chlorine isotope matching on molecular ion clusters.
- This approach uses allows “identity-blind” focus on chlorine and/or bromine-containing compounds in samples.
- Spectral library matches were available for only 18 “Cl”-pattern matched compounds in the SF Bay sample set.
- Most of these compounds were pharmaceuticals and/or agrochemicals.

Compound Discoverer 2.1.0.323

File Reporting Libraries View Window Help

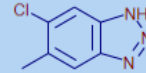
Start Page x SFEL_2017_0324 x

Compounds Compounds per File Merged Features Features mzVault Results mzCloud Results ChemSpider Results Mass List Search Results Input Files

	Checked	Name	Formula	Predicted Compositions* mzCloud Search mzVault Search ChemSpider Search MassList Match	Molecular Weight	RT [min]	# MS2	Area (Max.)	Pattern Matches	mzCloud Best Match	# mzCloud Results	# ChemSpider Results
1	<input type="checkbox"/>	Myclobutanil	C15 H17 Cl N4	■■■■■	288.11446	28.960	5	56539079	■ ■ ■ ■ ■	81.4	1	14
2	<input type="checkbox"/>	Phenol, 2,2'-thiobis[4-tert-butyl-	C20 H26 O2 S	■ ■ ■ ■ ■	330.16526	13.652	5	3753773	■ ■ ■ ■ ■	57.2	2	7
3	<input type="checkbox"/>	Losartan	C22 H23 Cl N6 O	■ ■ ■ ■ ■	422.16199	21.611	8	3195331	■ ■ ■ ■ ■	87.6	1	5
4	<input type="checkbox"/>	Losartan	C22 H23 Cl N6 O	■ ■ ■ ■ ■	422.16291	22.043	3	1258201	■ ■ ■ ■ ■	68.2	1	1
5	<input type="checkbox"/>	Losartan	C22 H23 Cl N6 O	■ ■ ■ ■ ■	422.16229	21.192	6	839837	■ ■ ■ ■ ■	86.1	1	3
6	<input type="checkbox"/>	Losartan	C22 H23 Cl N6 O	■ ■ ■ ■ ■	422.16201	22.062	2	700336	■ ■ ■ ■ ■	84.9	1	7
7	<input type="checkbox"/>	Clindamycin	C18 H33 Cl N2 O5 S	■ ■ ■ ■ ■	424.17984	15.238	6	393633	■ ■ ■ ■ ■	99.8	1	13
8	<input type="checkbox"/>	6-Chloro-5-methyl-1H-1,2,3-benzotriazole	C7 H6 Cl N3	■■■■■	167.02501	15.466	3	376255	■ ■ ■ ■ ■	79.6	3	100
9	<input type="checkbox"/>	Temazepam	C16 H13 Cl N2 O2	■■■■■	300.06639	22.242	12	352804	■ ■ ■ ■ ■	91.8	1	35
10	<input type="checkbox"/>	Clopidogrel carboxylic acid	C15 H14 Cl N O2 S	■ ■ ■ ■ ■	307.04332	10.068	5	301450	■ ■ ■ ■ ■	95.3	1	24
11	<input type="checkbox"/>	4-Chloro-N-[5-(2-methyl-2-propenyl)-	C14 H15 Cl N2 O2	■ ■ ■ ■ ■	278.08228	10.826	4	267665	■ ■ ■ ■ ■	50.4	1	25
12	<input type="checkbox"/>	Fenofibric acid	C17 H15 Cl O4	■ ■ ■ ■ ■	318.06572	30.088	1	255075	■ ■ ■ ■ ■	68.0	1	25
13	<input type="checkbox"/>	Phenol, 2,2'-thiobis[4-tert-butyl-	C20 H26 O2 S	■ ■ ■ ■ ■	330.16594	7.349	1	135556	■ ■ ■ ■ ■	59.4	2	15
14	<input type="checkbox"/>	Clindamycin	C18 H33 Cl N2 O5 S	■ ■ ■ ■ ■	424.17967	14.977	1	131760	■ ■ ■ ■ ■	97.3	1	2
15	<input type="checkbox"/>	Brilliant blue FCF	C37 H36 N2 O9 S3	■ ■ ■ ■ ■	748.15797	18.072	1	122568	■ ■ ■ ■ ■	85.8	1	1
16	<input type="checkbox"/>	Acamprosate	C5 H11 N O4 S	■ ■ ■ ■ ■	181.04070	19.579	2	119509	■ ■ ■ ■ ■	69.7	1	24
17	<input type="checkbox"/>	PIQUIZIL	C19 H26 N4 O4	■ ■ ■ ■ ■	374.19548	18.505	2	94898	■ ■ ■ ■ ■	50.9	1	7
18	<input type="checkbox"/>	Metoclopramide	C14 H22 Cl N3 O2	■ ■ ■ ■ ■	299.14025	9.989	3	70759	■ ■ ■ ■ ■	85.1	1	3

Hide Related Tables

Structure Proposals Compounds per File Predicted Compositions Merged Features Matched Patterns mzVault Results mzCloud Results ChemSpider Results Mass List Search Results

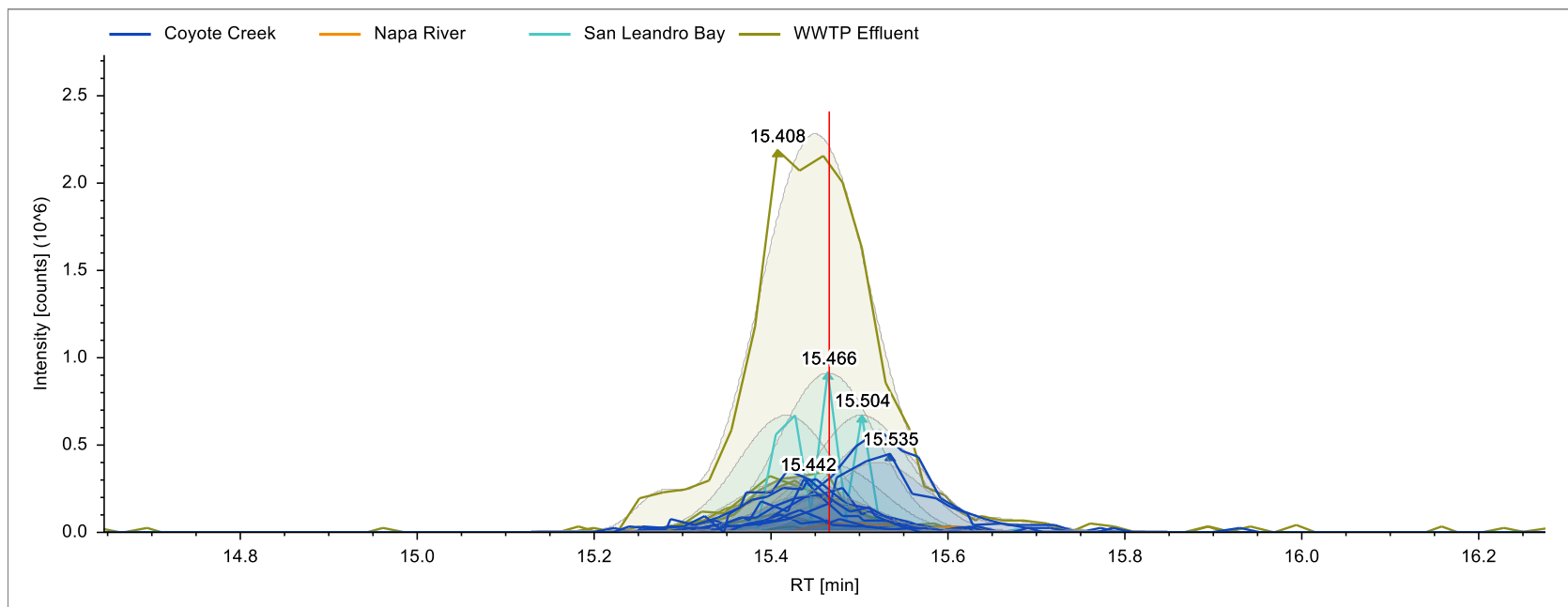
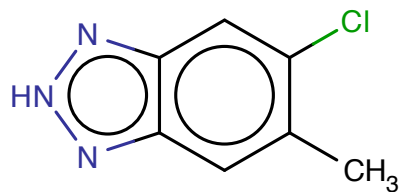
	Checked	Compound	ΔMass [Da]	ΔMass [ppm]	Scan Number	mzCloud ID	Formula	Structure	Molecular Weight	Match	Best Match	Name
1	<input type="checkbox"/>	<input checked="" type="checkbox"/>	0.00002	0.10	1812	3729	C7 H6 Cl N3		167.02502	79.6	79.6	6-Chloro-5-methyl-1H-1,2,3-benzotriazole

Show Related Tables

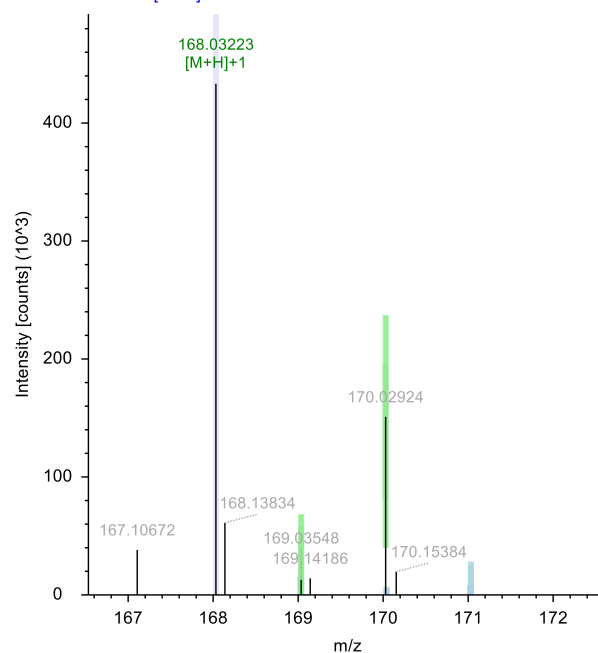
23

6-Chloro-5-methyl-1H-1,2,3-benzotriazole:

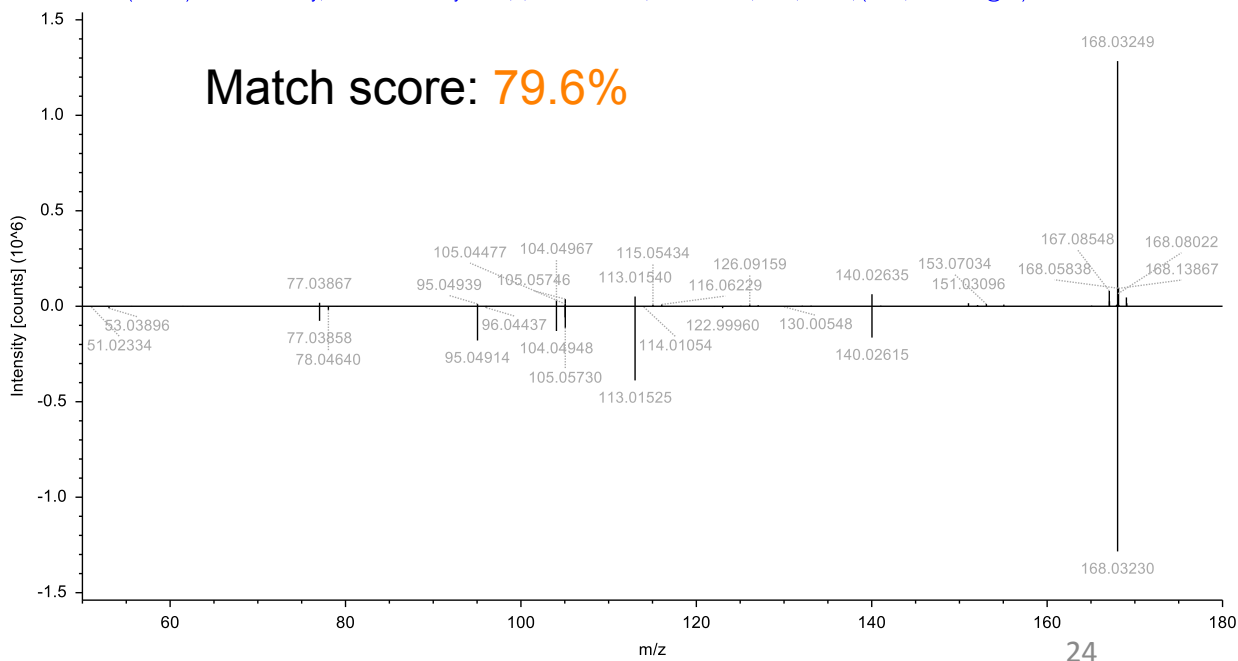
Chlorinated benzotriazoles are used in polymer additive UV inhibitors. This may be a precursor or transformation product of such polymer additives.



POCIS_CCP03_pos (F30) #1810, RT=15.535 min, MS1, FTMS (+)
C7 H6 Cl N3 as [M+H]⁺1



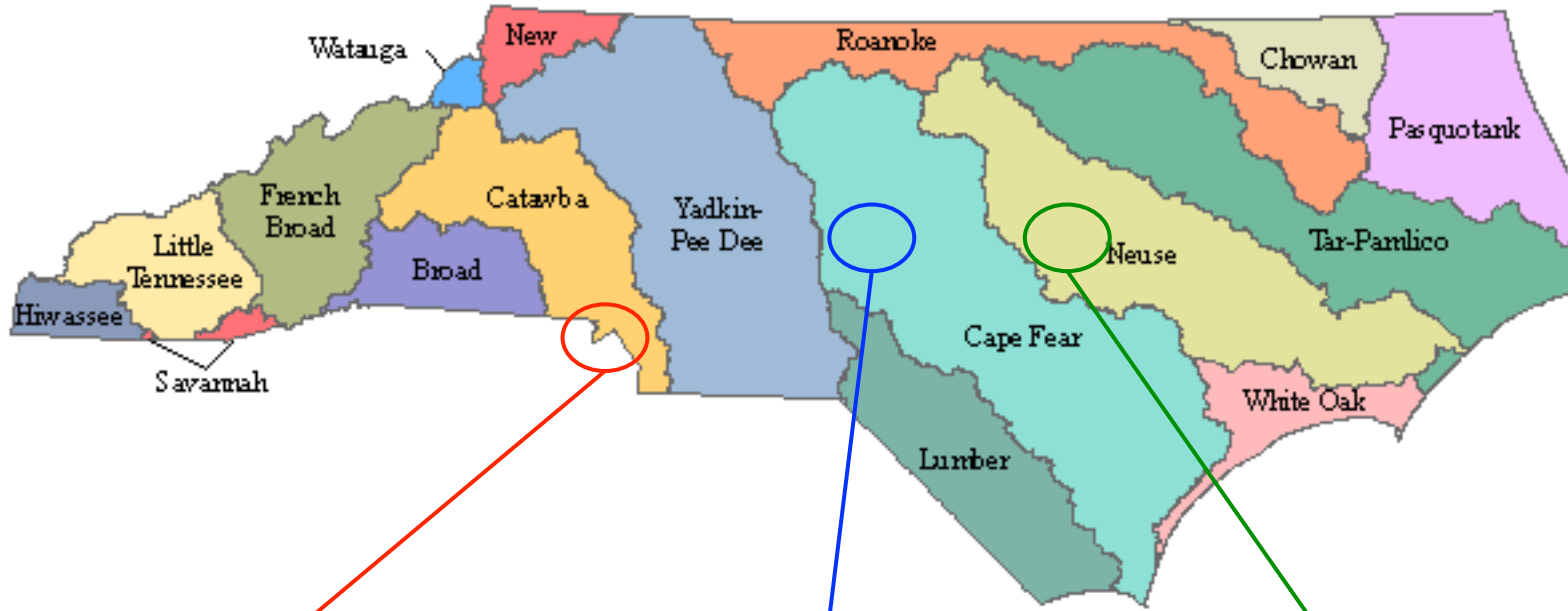
RAWFILE(top): POCIS_CCP03_pos (F30) #1812, RT=15.553 min, MS2, FTMS (+), (HCD, DDF, 168.0322@45, +1)
REFERENCE(bottom): mzCloud library, 6-Chloro-5-methyl-1H-1,2,3-benzotriazole, C7 H6 Cl N3, MS2, FTMS, (HCD, 168.0323@50)



Conclusions: SF Bay

- Bay waters are impacted by a variety of organic pollutant sources.
- Stormwater seems to be an important contributor of organic organic pollutant burdens in some areas of the Bay, as illustrated by findings of abundant polyethoxylated compounds and additive chemicals in San Leandro Bay.
- Agrochemicals and natural products appear to be the organic compounds most specifically detected in the Napa River.
- Passive sampling and discrete grab-sampling are complementary approaches for non-targeted analysis of ambient waters.

Emerging pollutants in NC river water

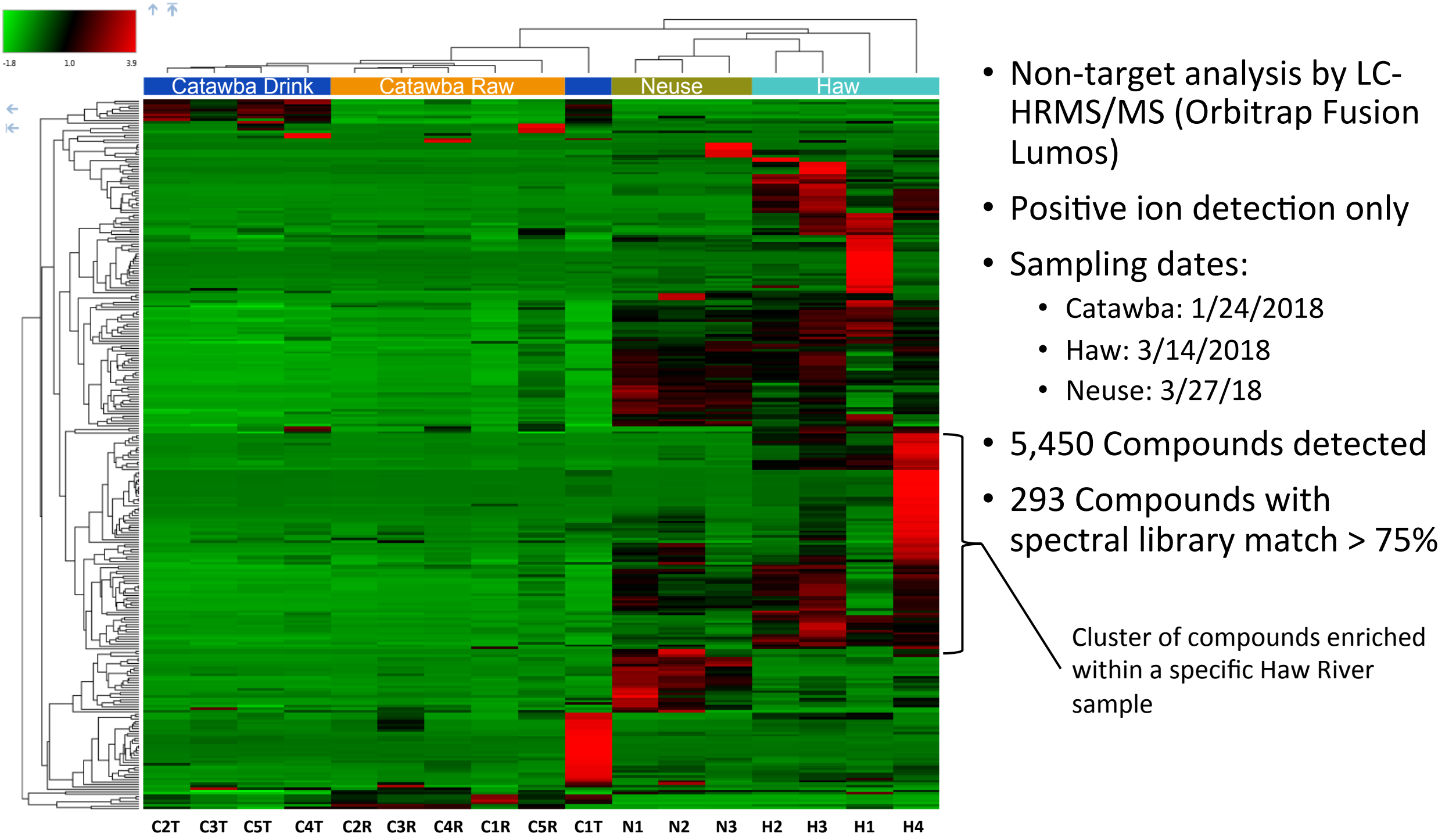


Catawba river: highly urbanized, significant wastewater inputs. Drinking water source for Charlotte, NC Metro area

Haw river: within the Cape Fear watershed. Industry and urbanization are likely pollution sources.

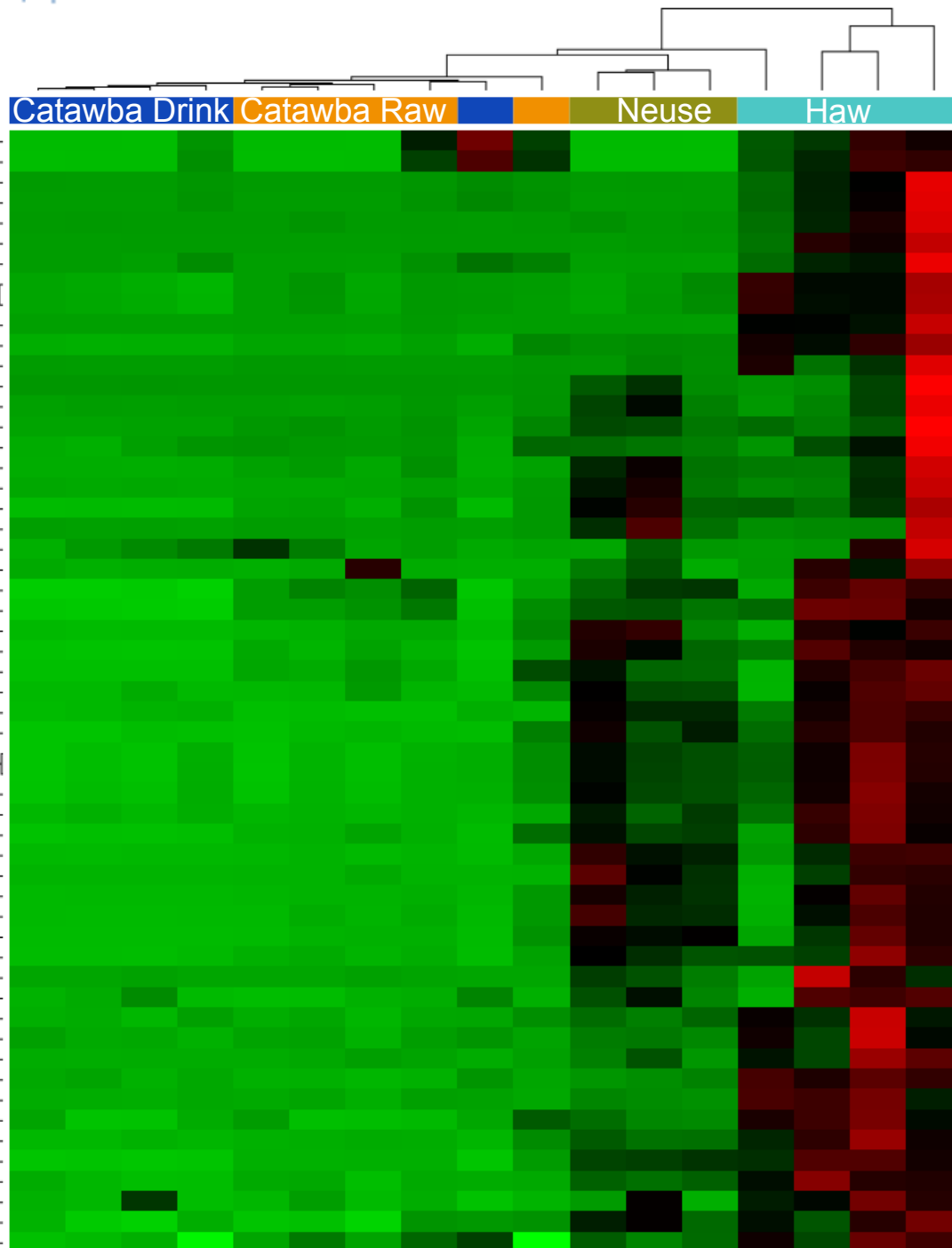
Neuse river: agriculture is the dominant land-use. Tobacco, corn, hog farms ubiquitous throughout watershed.

- Discovery of GenX (next-generation PFOA replacement chemical) at high levels in drinking water downstream of a manufacturer on the Cape Fear river has heightened awareness of emerging pollutants in NC waters.
- Collaboration with non-profit riverkeeper alliances and EPA NERL (RTP) established to perform emerging contaminant reconnaissance.
- Initial non-targeted analysis work has focused on source (raw) and treated (drinking) waters in three basins within NC.

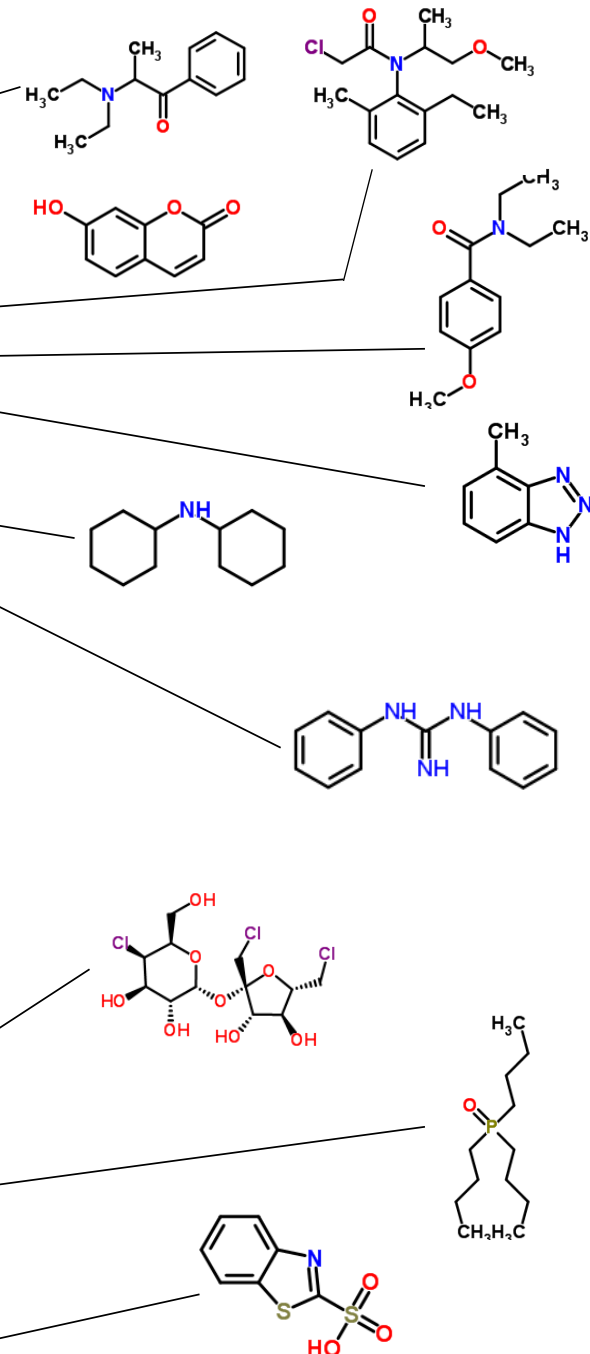




-1.4 1.1 3.7

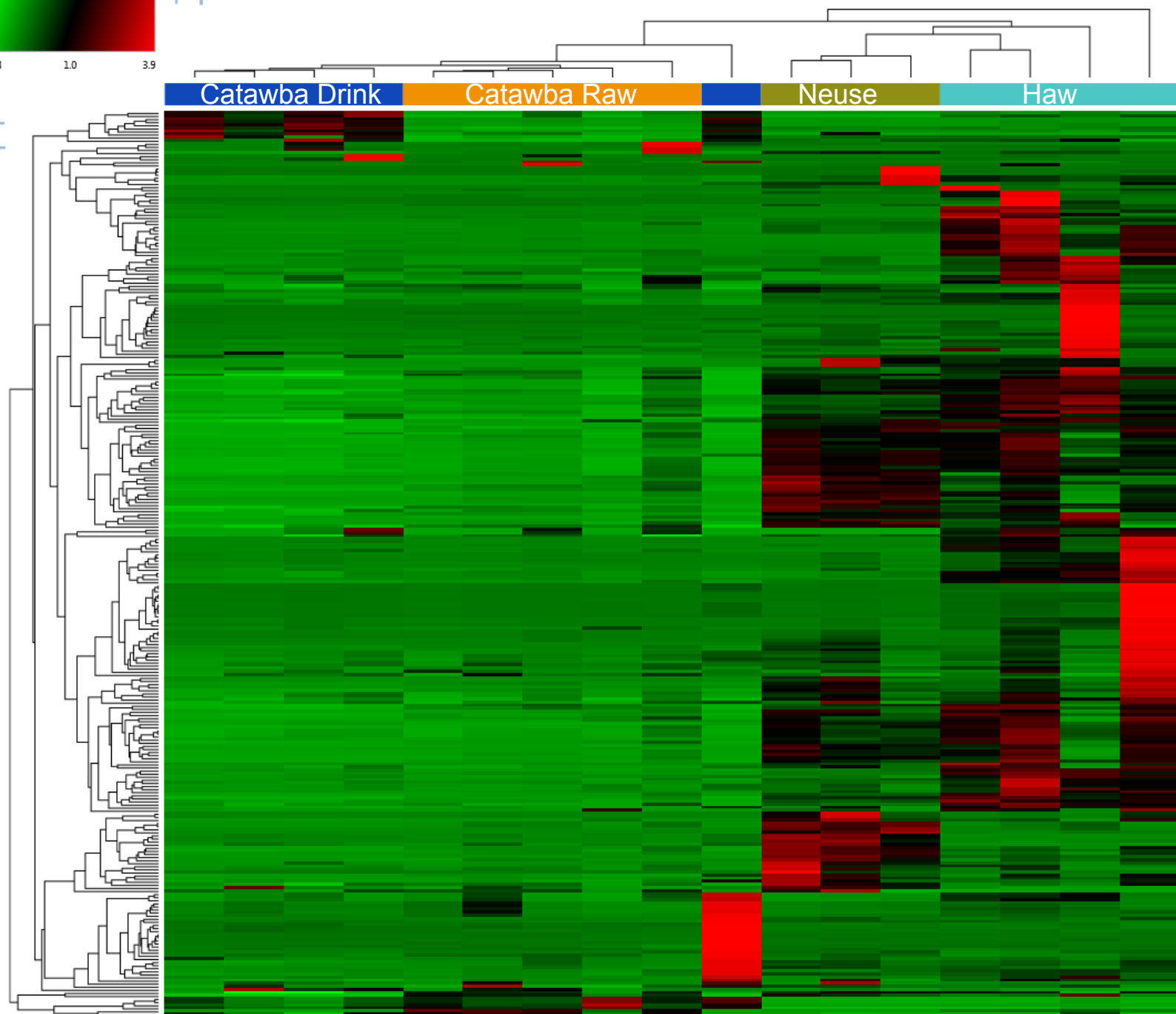


N,N-Diethylcathinone, MW: 205.14...
Amfepramone, MW: 205.14667, RT: 2...
1,5-Isoquinolinediol, MW: 161.047...
1H-Indole-2-carboxylic acid, ethyl...
N-Ethyl-4-methoxybenzamide, M...
7-Hydroxycoumarin, MW: 162.03...
1,5-Isoquinolinediol, MW: 161.047...
Metolachlor, MW: 251.10775, RT: 2...
Metolachlor, MW: 283.13395, RT: 2...
N,N-Diethyl-4-methoxybenzamide,...
4-Methylbenzotriazole, MW: 133.0...
Metaxalone, MW: 160.08887, RT: 2...
4-Nitrosodiphenylamine, MW: 198...
N-Cyclohexyl-2-benzothiazol-amin...
Tributylamine, MW: 185.21428, RT: 2...
Dicyclohexylamine, MW: 181.18308...
N,N'-Diphenylguanidine, MW: 211...
N-Hexanoyl-DL-homoserine lacton...
Phenamil, MW: 135.07965, RT: 2.053
Indaziflam, MW: 301.17025, RT: 18...
Diethyl sulfosuccinate, MW: 466.19...
Glaucine, MW: 355.17830, RT: 11.861
8-Hydroxyquinoline, MW: 145.052...
Dimethylaminopurine, MW: 163.08...
Carbamazepine 10,11-epoxide, M...
Riboflavin, MW: 376.13835, RT: 7.353
2-Ethylidene-1,5-dimethyl-3,3-dip...
Methadone, MW: 309.20918, RT: 1...
2-(3,4-Dimethoxyphenyl)-5-methyl...
Atenolol, MW: 266.16312, RT: 3.637
10-Hydroxycarbamazepine, MW: 254...
Carbamazepine, MW: 236.09502, R...
Iminostilbene, MW: 193.08918, RT: 5...
Doxylamine, MW: 181.08917, RT: 5...
Oxycodone, MW: 315.14714, RT: 5...
Levamisole, MW: 204.07219, RT: 5...
4-Hydroxyomeprazole sulfide, MW...
Sitagliptin, MW: 407.11809, RT: 10...
Triamterene, MW: 253.10768, RT: 7...
Ranolazine, MW: 427.24691, RT: 13...
N-Ethylamphetamine, MW: 163.13...
Stercobilin, MW: 594.34254, RT: 14...
2-Hydroxyquinoline, MW: 145.052...
Sucralose, MW: 417.99666, RT: 6.607
4-Hydroxyindole, MW: 133.05280,...
Piperine, MW: 285.13660, RT: 21.217
Tributylphosphine oxide, MW: 218...
5-Methoxyindole, MW: 147.06846,...
4-Methoxycinnamaldehyde, MW: 1...
Methocarbamol, MW: 241.09521, R...
.beta.-Carboline-1-propionic acid,...
Atraton, MW: 211.14333, RT: 7.152
Dodecyltrimethylammonium, MW:...
2-Benzothiazolesulfonic acid, MW:...
5,6-Dimethylbenzimidazole, MW: 1...





-1.8 1.0 3.9



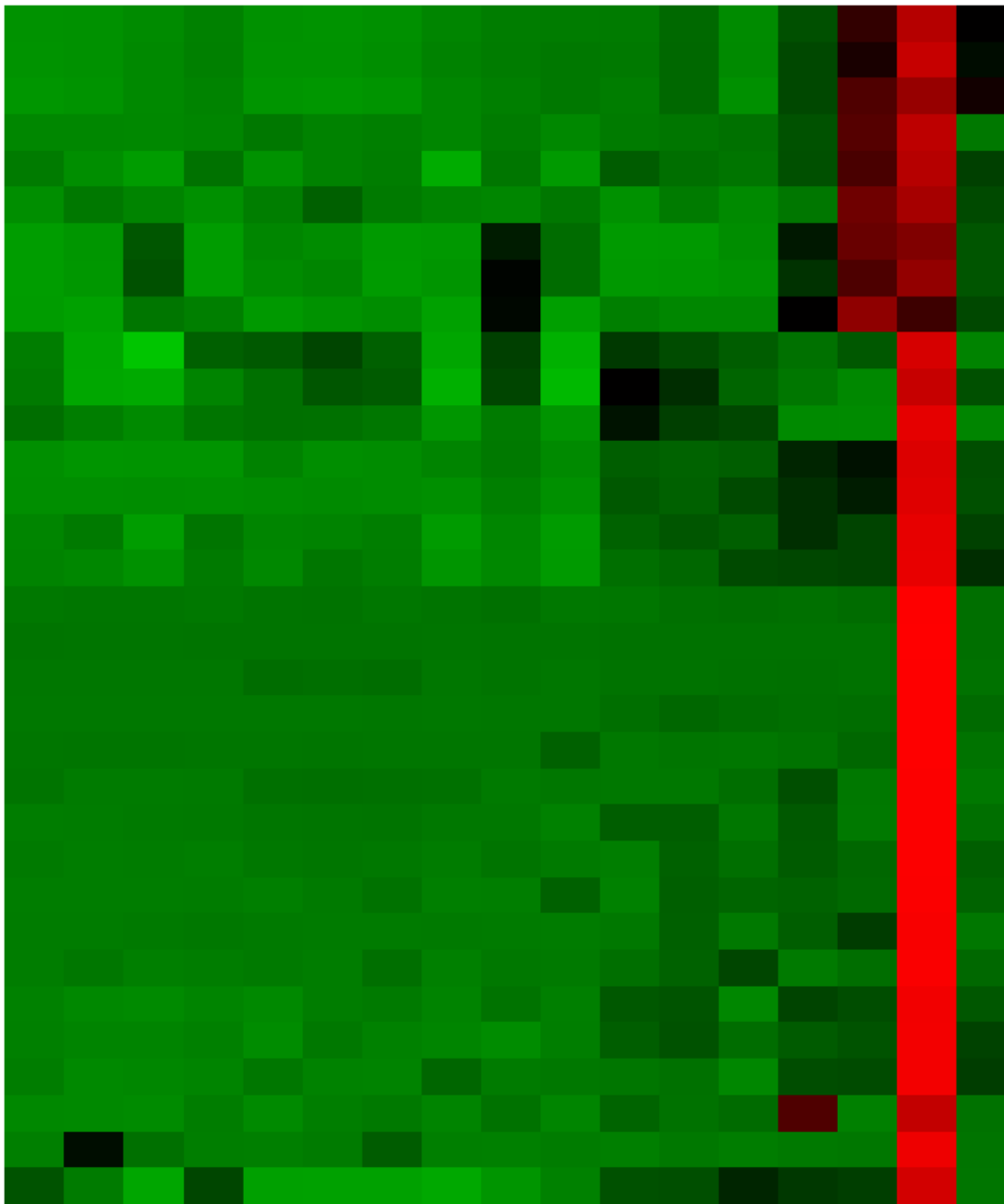
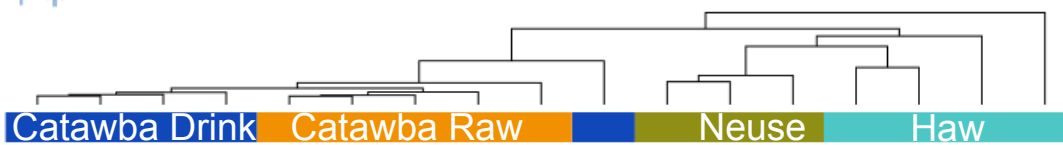
Catawba Drink

Catawba Raw

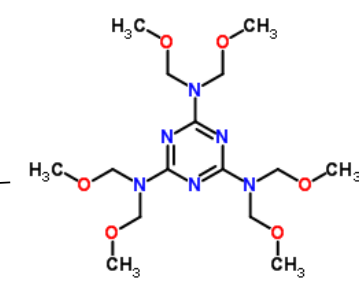
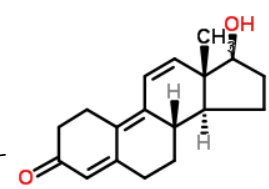
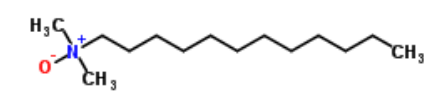
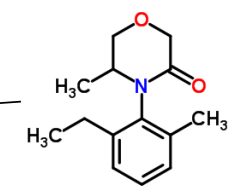
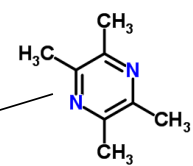
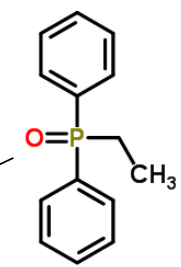
Neuse

Haw

C2T C3T C5T C4T C2R C3R C4R C1R C5R C1T N1 N2 N3 H2 H3 H1 H4

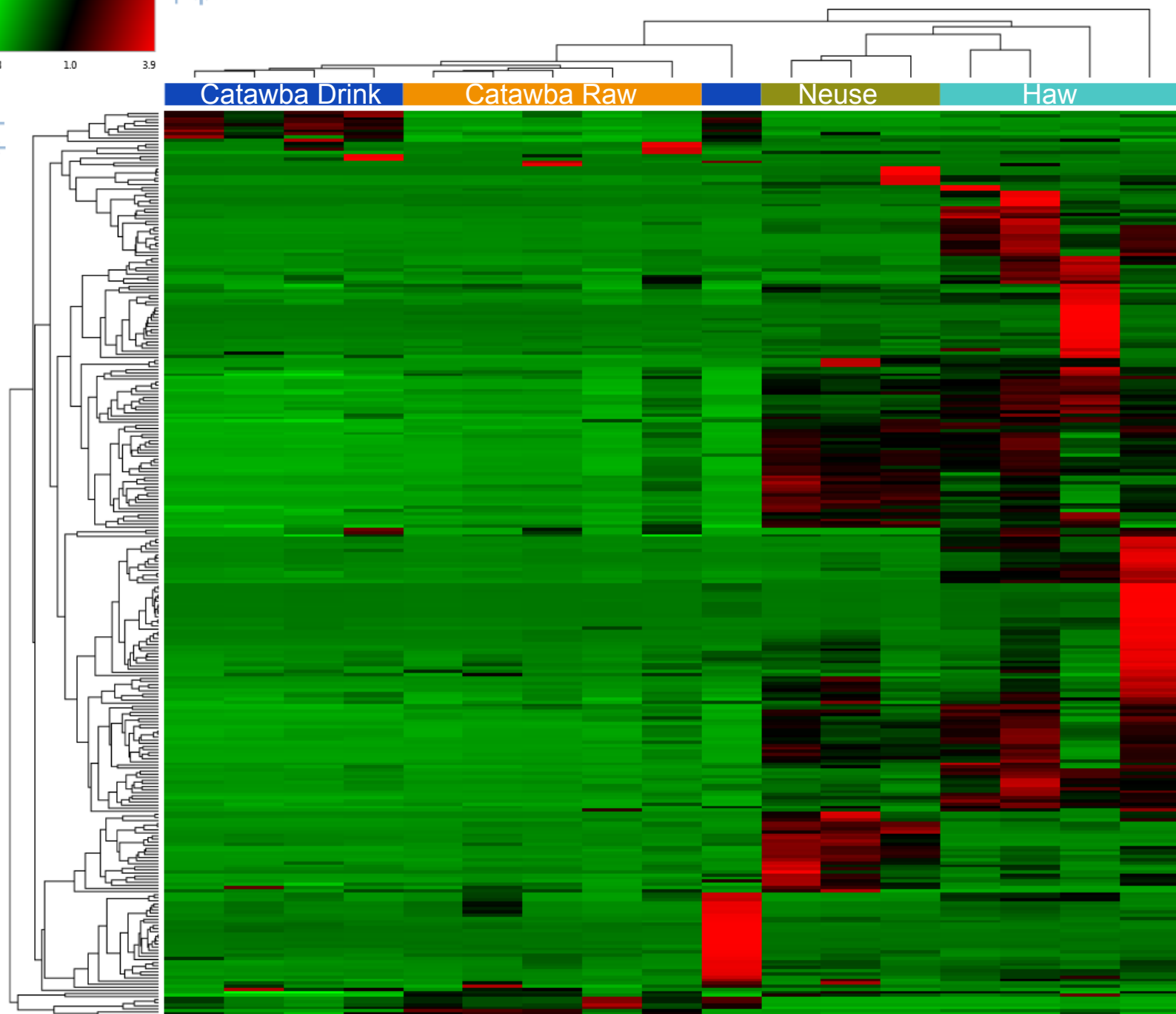


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 PEG n14, MW: 651.40526, RT: 8.915
 PEG n12, MW: 563.35241, RT: 8.071
 Indole-3-acrylic acid, MW: 187.063...
 5-Methoxyindole, MW: 147.06847,...
 PEG Monolaurate n4, MW: 398.264...
 Carvyl acetate, MW: 134.10960, RT:...
 2,4,7,9-Tetramethyl-5-decyne-4,7-...
 Ethyldiphenylphosphine oxide, M...
 Pyroquilon, MW: 173.08415, RT: 3.4...
 5-Phenylcyclohexane-1,3-dione, M...
 N-Methyl-L-phenylalanine, MW: 13...
 2,3,5,6-Tetramethylpyrazine, MW:...
 Norlidocaine, MW: 206.14189, RT:...
 Metolachlor morpholinone, MW: 2...
 Metolachlor morpholinone, MW: 2...
 Dehydroepiandrosterone (DHEA),...
 Echinocystic acid, MW: 436.33406,...
 Indolmycin, MW: 257.11647, RT: 12...
 Isotretinoin, MW: 300.20893, RT: 2...
 N,N-Dimethyldodecylamine N-oxi...
 5-Androstene-3.beta.,17.beta.-diol,...
 Dehydroepiandrosterone (DHEA),...
 (+/-)-12-HpETE, MW: 318.21946, RT...
 Kahweol, MW: 314.18813, RT: 24.470
 10-Nitrolinoleate, MW: 325.22523,...
 Trenbolone, MW: 252.15146, RT: 1...
 Kahweol, MW: 314.18817, RT: 17.353
 Dehydroepiandrosterone (DHEA),...
 Hexamethoxymethyl melamine, M...
 1-Methylbenzotriazole, MW: 133.0...
 Eicosapentaenoic acid, MW: 302.22...
 α,α-Diphenyl-4-piperidinomethan...





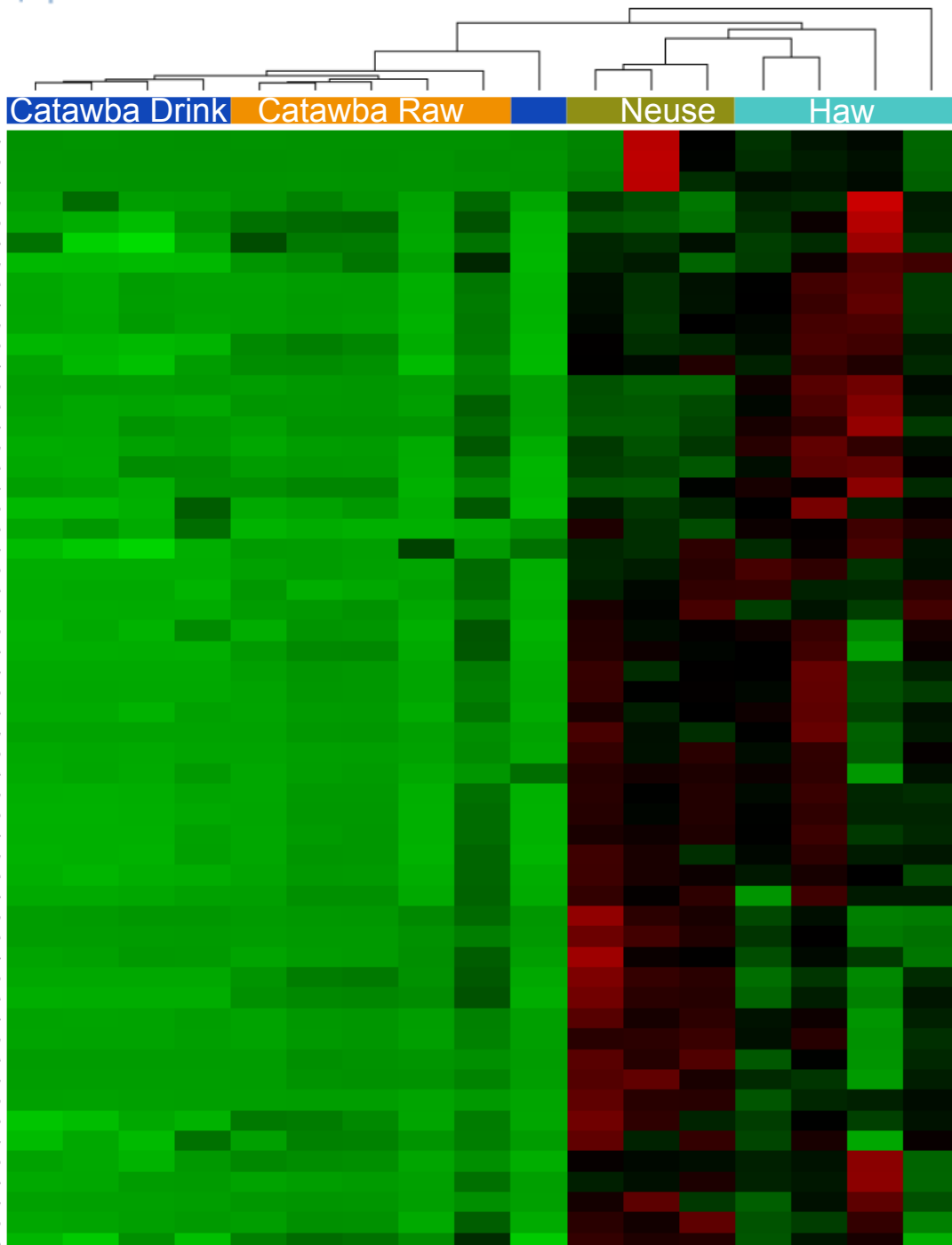
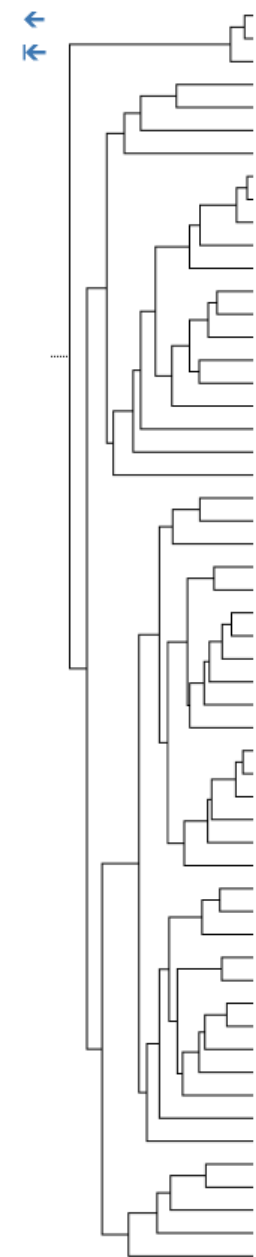
-1.8 1.0 3.9



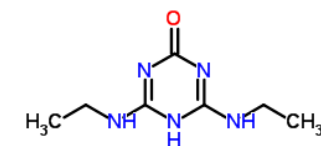
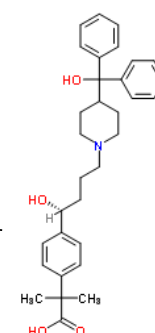
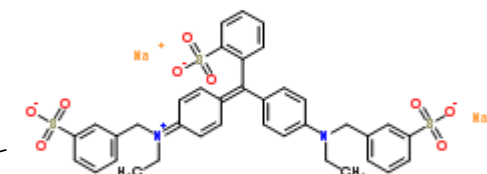
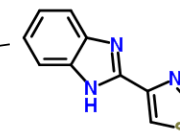
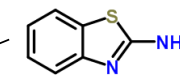
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-1.8 1.0 3.9

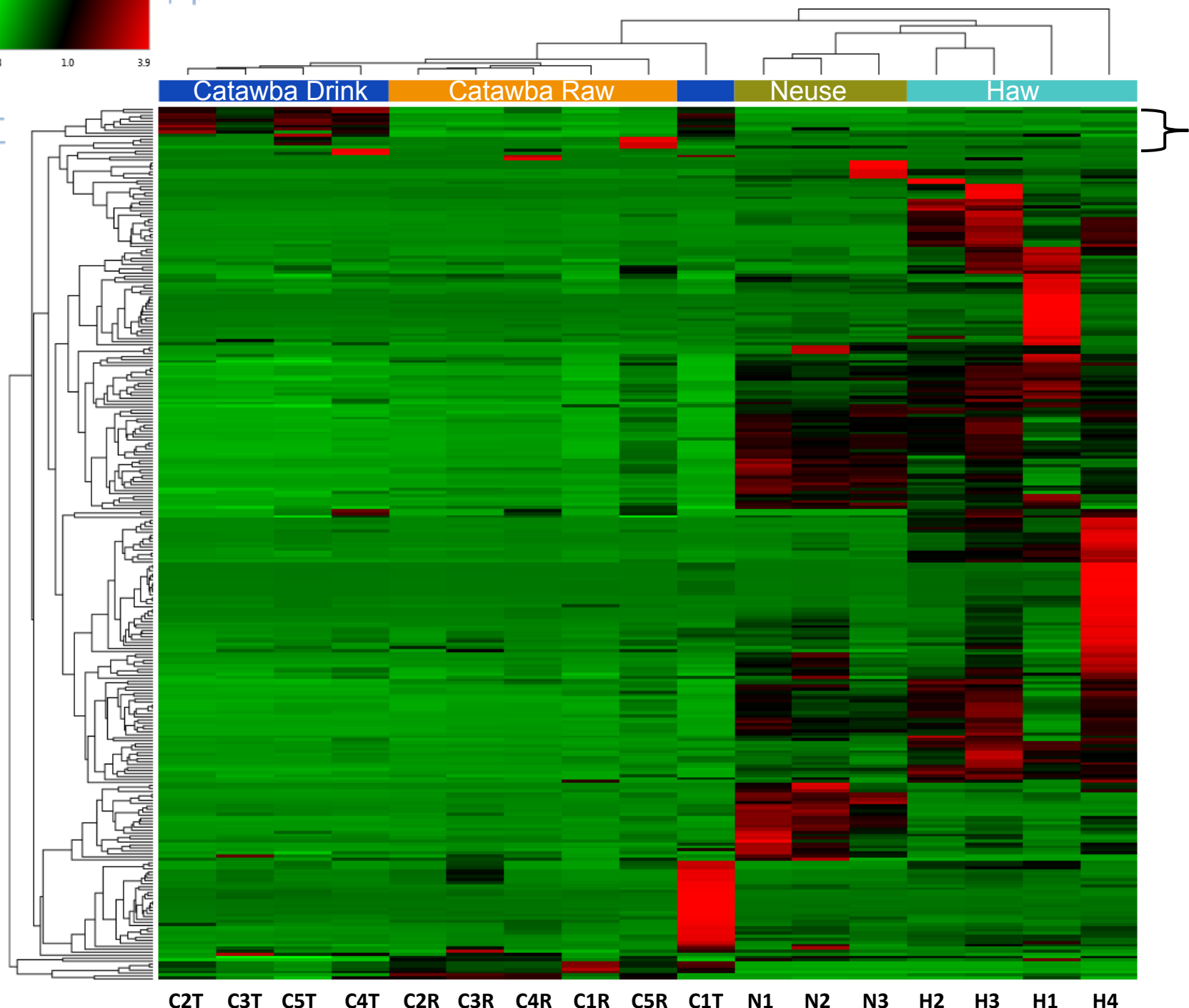


9-Oxo-10(E),12(E)-octadecadienoic...
 9-Oxo-10(E),12(E)-octadecadienoic...
 9-Oxo-10(E),12(E)-octadecadienoic...
 Triethyl phosphate, MW: 182.0708...
 Benzoguanamine, MW: 187.08588...
 3,6-Dimethylchromone, MW: 174.0...
 2-Aminobenzothiazole, MW: 150.0...
 10,11-Dihydro-10,11-dihydroxycar...
 Carbamazepine 10,11-epoxide, M...
 Acridine, MW: 179.07356, RT: 9.601
 2-Methyl-3-(2',3'-dihydroxypropyl)...
 (3R,3aR,4R,4aR,7aR,8R,9aR)-3,4a,8-...
 Thiabendazole, MW: 201.03609, RT...
 2-Isopropyl-6-methyl-4-pyrimidino...
 Gabapentin related compound A,...
 Temazepam, MW: 300.06653, RT: 1...
 Lauro lactam, MW: 197.17798, RT: 1...
 2-Hydroxyatrazine, MW: 197.12770...
 Lidocaine, MW: 234.17328, RT: 7.187
 Desmethylocitalopram, MW: 310.14...
 Clopidogrel carboxylic acid, MW: 3...
 Olmesartan, MW: 446.20671, RT: 1...
 Brilliant blue FCF, MW: 748.15966...
 Flecainide, MW: 414.13791, RT: 15...
 Venlafaxine, MW: 277.20419, RT: 1...
 Fexofenadine, MW: 501.28817, RT:...
 Fexofenadine, MW: 483.27758, RT:...
 Telmisartan, MW: 514.23744, RT: 1...
 Losartan, MW: 422.16292, RT: 16.415
 10-Hydroxycarbazepine, MW: 254...
 .beta.-Estradiol, MW: 272.17770, R...
 threo-dihydrobupropion, MW: 241...
 rac erythro-Dihydrobupropion, M...
 rac erythro-Dihydrobupropion, M...
 3-Amino-2-(4-chlorophenyl)-2-hyd...
 2-Quinoxalinecarboxamide, N-tricy...
 rac erythro-Dihydrobupropion, M...
 Valsartan, MW: 435.22709, RT: 19.9...
 Valsartan, MW: 457.20928, RT: 19.9...
 Losartancarboxaldehyde, MW: 206...
 O-Desmethylvenlafaxine, MW: 263...
 O-Desmethyltramadol, MW: 249.1...
 Bupropion, MW: 183.04516, RT: 11...
 Bupropion, MW: 239.10776, RT: 11...
 Zolpidem phenyl-4-carboxylic acid,...
 Carbamazepine 10,11-epoxide, M...
 N-(2,6-Dimethylphenyl)-N-(metho...
 N-Desmethyldiltiazem, MW: 400.1...
 Desacetyl diltiazem, MW: 372.1507...
 2-Hydroxysimazine, MW: 183.1120...
 Tetranor-12(S)-HETE, MW: 248.177...
 Azoxystrobin acid, MW: 389.10115...
 Tetranor-12(S)-HETE, MW: 248.177...
 Gabapentin related compound A,...





-1.8 1.0 3.9



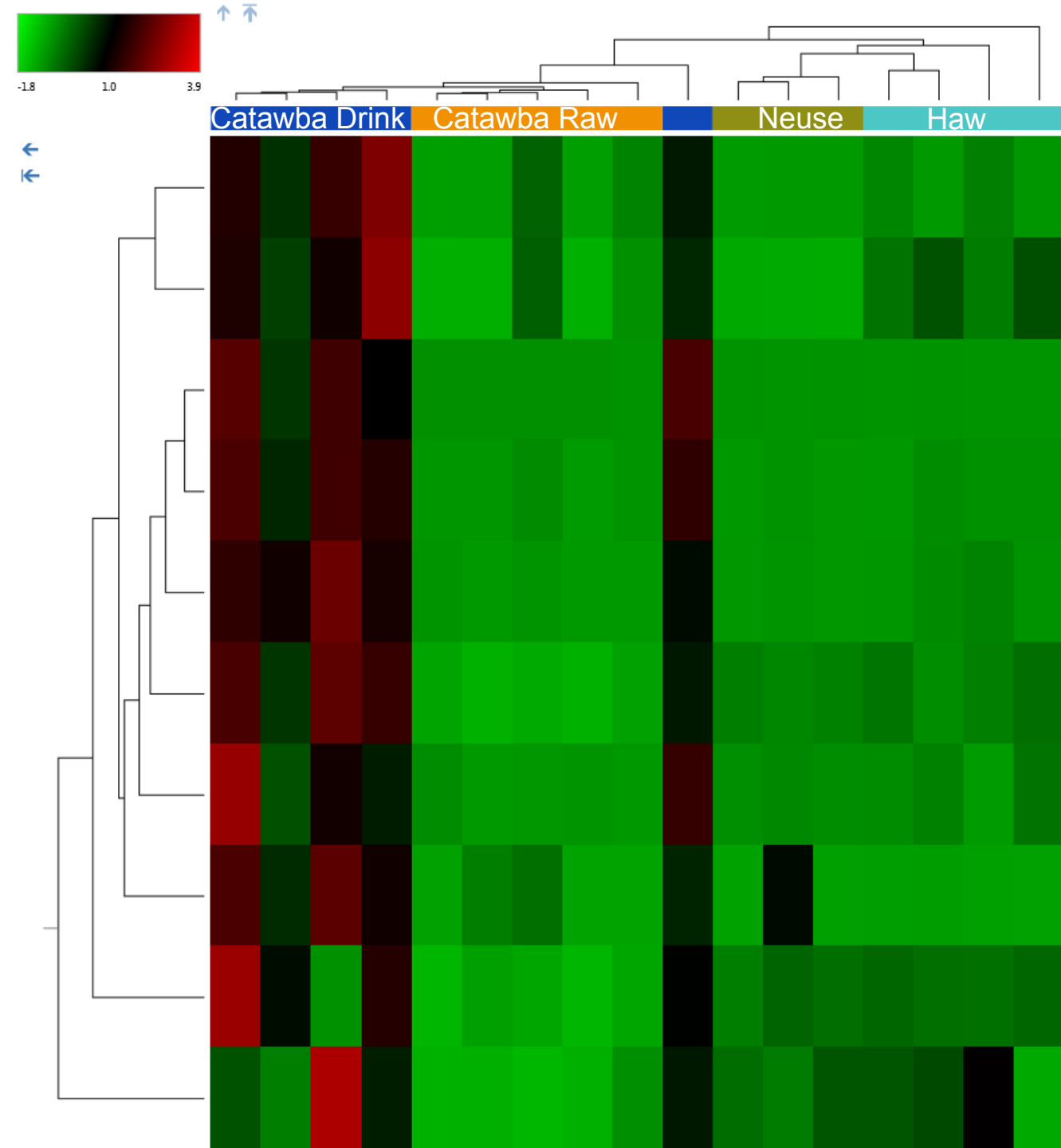
Catawba Drink

Catawba Raw

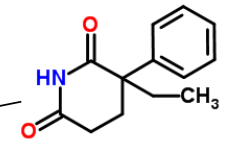
Neuse

Haw

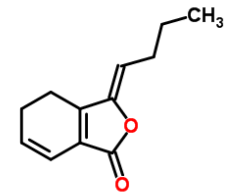
C2T C3T C5T C4T C2R C3R C4R C1R C5R C1T N1 N2 N3 H2 H3 H1 H4



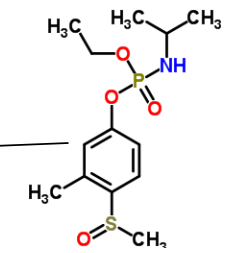
Glutethimide, MW: 172.08884, RT:...



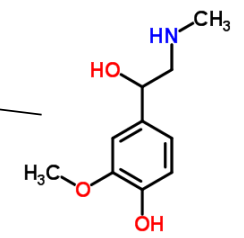
Z-Ligustilide, MW: 172.08884, RT: 1...



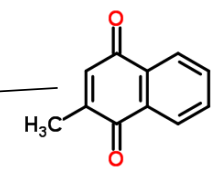
Fenamifos sulfoxide, MW: 291.068...



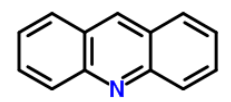
Glutethimide, MW: 189.11540, RT:...



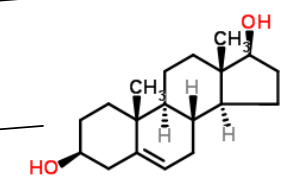
Metanephrine, MW: 197.10522, RT:...



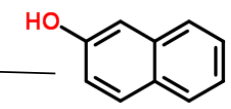
Menadione, MW: 144.05755, RT: 1...



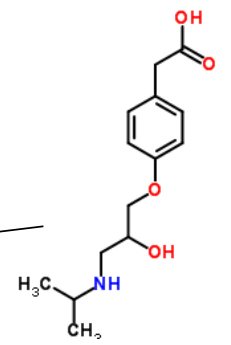
Acridine, MW: 179.07355, RT: 7.688



5-Androstene-3.beta.,17.beta.-diol,...



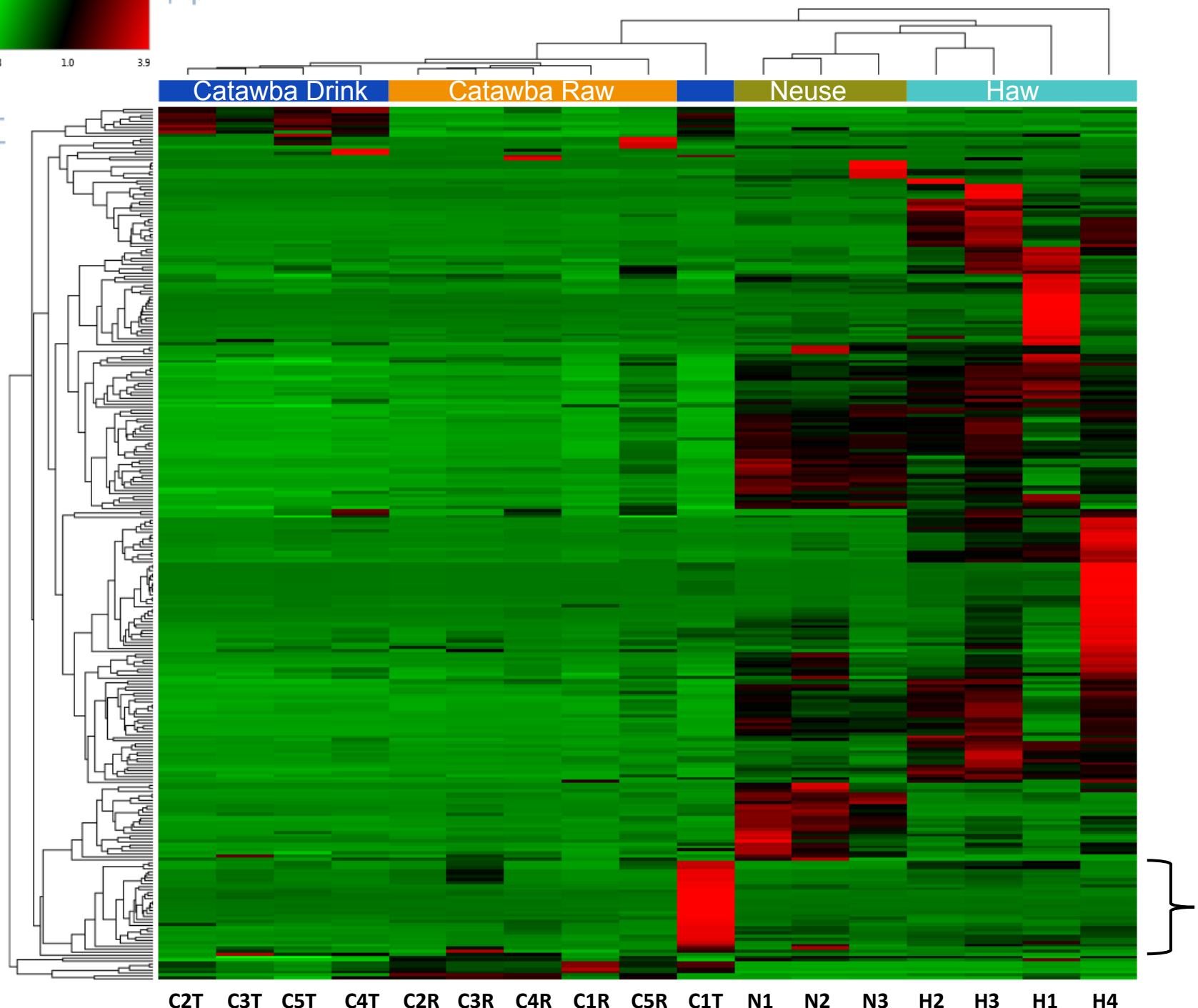
.beta.-Naphthol, MW: 144.05754, R...



Metoprolol acid, MW: 267.14717, R...



-1.8 1.0 3.9



Catawba Drink

Catawba Raw

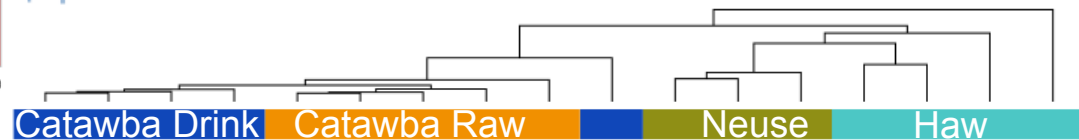
Neuse

Haw

C2T C3T C5T C4T C2R C3R C4R C1R C5R C1T N1 N2 N3 H2 H3 H1 H4



-1.8 1.0 3.9

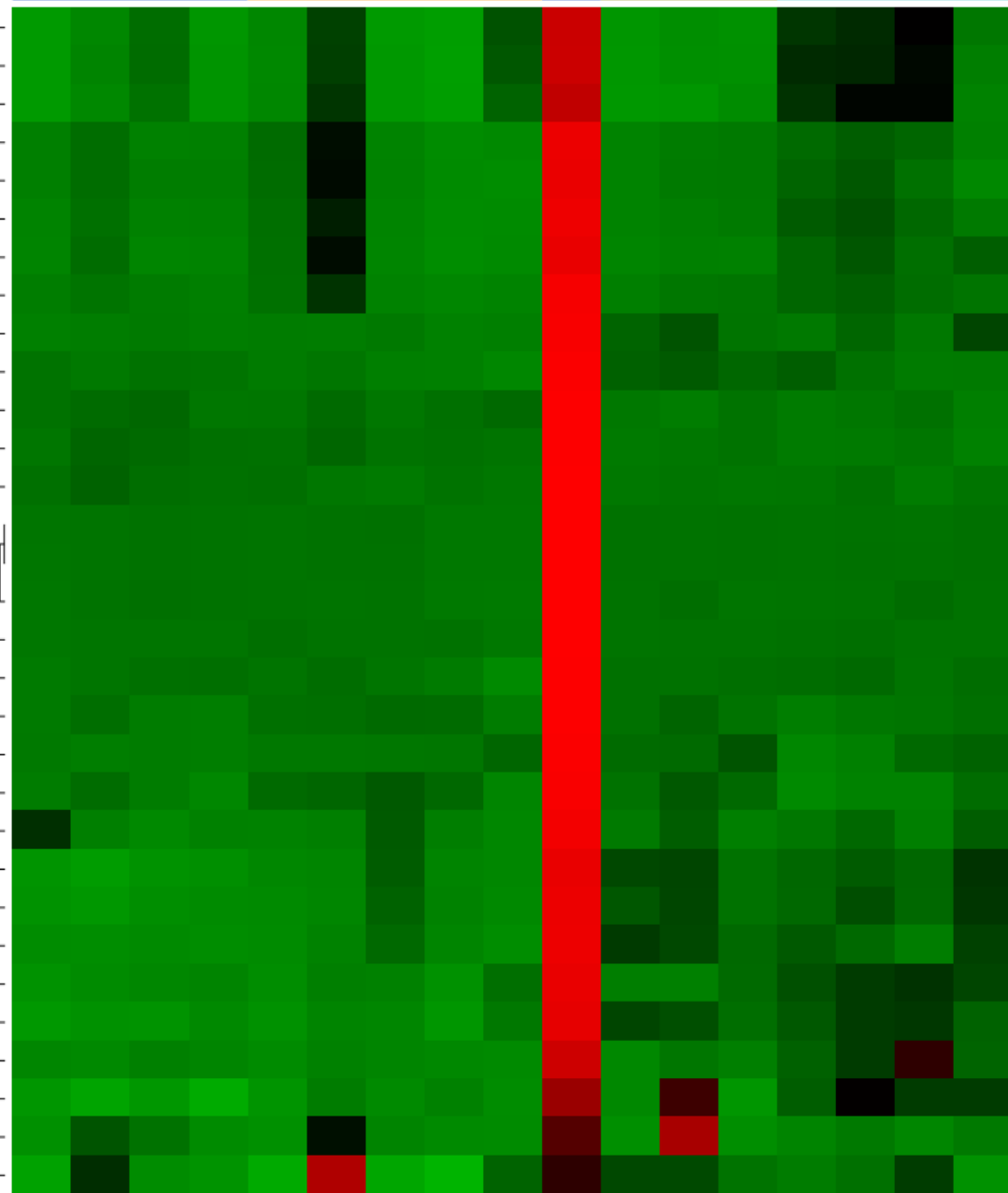


Catawba Drink

Catawba Raw

Neuse

Haw



2,4,7,9-Tetramethyl-5-decyne-4,7-...

2,4,7,9-Tetramethyl-5-decyne-4,7-...

(-)-Perillyl alcohol, MW: 134.10960,...

2,4,7,9-Tetramethyl-5-decyne-4,7-...

2,4,7,9-Tetramethyl-5-decyne-4,7-...

Decynediol, tetramethyl, di(2-hydr...

(-)-Perillyl alcohol, MW: 134.10959,...

Decynediol, tetramethyl, di(2-hydr...

Triphenyl phosphate, MW: 326.070...

Phthalic anhydride, MW: 148.0160...

Dibutyl sebacate, MW: 314.24569,...

Hexadecanamide, MW: 255.25627,...

N,N-Dimethyldodecylamine N-oxi...

α -Linolenic acid, MW: 278.22459, R...

9,10-Dihydroxy-12Z-octadecenoic...

.gamma.-Linolenoyl ethanolamide,...

1-Dodecyl-2-pyrrolidinone, MW: 2...

3,5-di-tert-Butyl-4-hydroxybenzald...

Triethyleneglycol bis(2-ethylhexan...

α -Linolenic acid, MW: 278.22457, R...

Triethyleneglycol bis(2-ethylhexan...

Citroflex A-4, MW: 402.22532, RT: 2...

Decamethylcyclotrisiloxane, M...

Hexamethylcyclotrisiloxane, MW: 2...

Decamethylcyclotrisiloxane, M...

Tris(1-chloro-2-propyl)phosphate,...

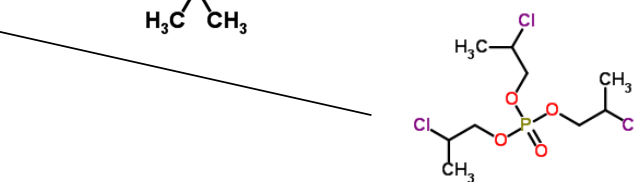
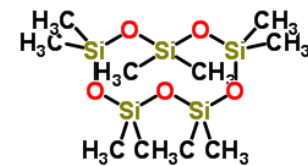
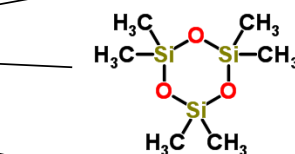
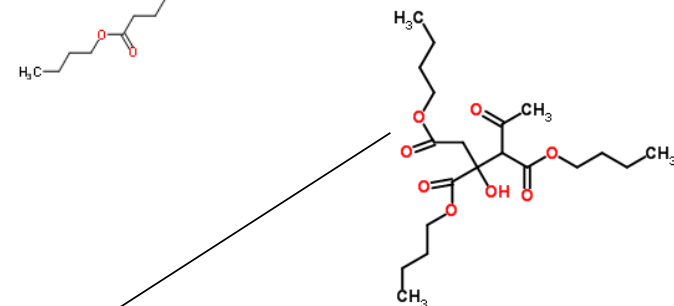
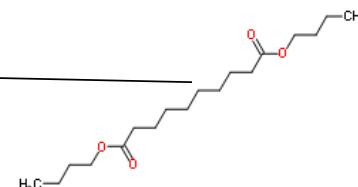
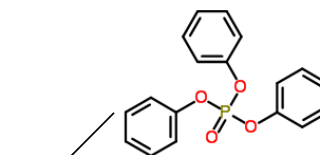
Tris(2-chloropropyl) phosphate, M...

1-Tetradecylamine, MW: 213.2456...

Bis(2-ethylhexyl) amine, MW: 241.2...

Benfluorex, MW: 148.05245, RT: 22...

Tributyl phosphate, MW: 266.1648...



Conclusions: NC River monitoring

- A wide range of unregulated emerging contaminants were detectable in river waters across the state of North Carolina.
- Abundant compounds in the Haw River watershed included markers of urban stormwater, including tire-related chemicals and polymer additives.
- The Neuse river showed evidence of agrochemical contamination, consistent with land-use practices in the watershed.
- Non-targeted analysis of paired raw/drinking water revealed disinfection byproducts and suspected piping-derived polymer additive chemicals in finished drinking waters.

Future directions

- Statistically-sound, comprehensive identification of organic pollutants in water using a harmonized workflow: *in silico* MS/MS and evidence-based prioritization (moving beyond library matching).
- Application of computational transformation product prediction from identified “leads” for drilling-down into possible pollutant TP identifications.
- Enhanced prioritization of compound identification using pairwise differential analysis among spatial and temporal samples.
- Annotation of compound identifications by molecular ontology, functional use, and toxicity data/predictions using open-source tools including EPA CompTox Dashboard.

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NC Riverkeepers Alliance

- Emily Sutton (Haw River)
- Sam Perkins (Catawba River)
- Matthew Starr (Neuse River)

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